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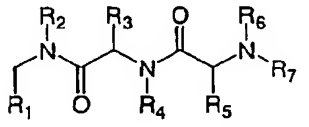
(71) Applicant: **CHUGAI SEIYAKU KABUSHIKI KAISHA**
Tokyo, 115-8543 (JP)

(72) Inventors:
- **SHIRAISHI, Takuya, c/o Chugai Seiyaku K.K. Gotenba-shi, Shizuoka 412-8513 (JP)**
- **KADONO, Shojiro, c/o Chugai Seiyaku K.K. Gotenba-shi, Shizuoka 412-8513 (JP)**
- **HARAMURA, Masayuki, c/o Chugai Seiyaku K.K. Gotenba-shi, Shizuoka 412-8513 (JP)**
- **SATO, Haruhiko c/o Chugai Seiyaku Kabushiki Kaisha Gotenba-shi, Shizuoka 412-8513 (JP)**
- **KOZONO, Toshiro, c/o Chugai Seiyaku K.K. Gotenba-shi, Shizuoka 412-8513 (JP)**
- **KOGA, Takaki, c/o Chugai Seiyaku Kabushiki Kaisha Gotenba-shi, Shizuoka 412-8513 (JP)**
- **SAKAMOTO, Akihisa, c/o Chugai Seiyaku K.K. Gotenba-shi, Shizuoka 412-8513 (JP)**

(74) Representative: **VOSSIUS & PARTNER**
Siebertstrasse 4
81675 München (DE)

(54) PEPTIDE DERIVATIVES

(57) A compound of Formula (1):



(1)

wherein
R_1 represents an amidinophenyl group, etc.;
R_2 represents a hydrogen atom, etc.;
R_3 represents a carbamoylalkyl group, etc.;
R_4 represents a hydrogen atom, etc.;
R_5 represents a benzyl group, etc.;
R_6 represents a hydrogen atom, etc.; and
R_7 represents an alkylsulfonyl group, etc.
A crystal of a complex between factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor. A medium carrying a part or all of structure coordinate data of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, obtainable by X-ray crystal structure analysis of the crystal. A method for computationally designing a low-molecular weight reversible factor VIIa inhibitor using the coordinate data.

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Description

TECHNICAL FIELD

[0001] The present invention relates to peptide derivatives having an inhibitory activity against blood coagulation factor VIIa.

BACKGROUND ART

[0002] Blood coagulation is a host defense mechanism provoked in response to vascular injury and/or foreign stimulation. Blood coagulation involves 15 factors including 12 proteinaceous coagulation factors in plasma, along with calcium ion, tissue factor and phospholipid (platelet-derived). This reaction is mediated by a cascade mechanism, in which a series of protease activations occurs successively on the membrane of platelets aggregated at a site of injury or damaged endothelial cells.

[0003] The blood coagulation cascade is divided into intrinsic and extrinsic pathways. It is called extrinsic blood coagulation when it occurs with the aid of tissue factor present in tissues, while it is called intrinsic blood coagulation when it occurs without the aid of tissue factor.

[0004] Intrinsic blood coagulation is initiated by the contact of blood coagulation factor XII in plasma with the surface of a negatively-charged solid phase or the like. Upon adsorption onto the surface, factor XII is converted through limited hydrolysis into activated factor XII (XIIa), an active protease. In turn, factor XIIa causes the limited hydrolysis of factor XI into activated factor XI (XIa), an active protease. After such a cascade of protease activations, the final protease thrombin causes the limited hydrolysis of fibrinogen into fibrin, leading to the completion of blood coagulation. In downstream reactions after the activation of factor XI, a number of coagulation factors are assembled into complexes to facilitate coagulation factor localization at a site of hemostasis and to ensure efficient activation reactions. Namely, a tenase complex is assembled from phospholipids, factor VIIIa, factor IXa, factor X and Ca^{2+}, while a prothrombinase complex is assembled from phospholipids, factor Va, factor Xa, prothrombin and Ca^{2+}, resulting in significant promotion of prothrombin activation.

[0005] Extrinsic blood coagulation is initiated by the formation of a complex between factor VIIa and tissue factor. This complex between factor VIIa and tissue factor will join the intrinsic pathway at the stage of factor X and IX activation.

[0006] In general, extrinsic blood coagulation is reported to be important for hypercoagulation and physiological coagulation under pathological conditions.

[0007] Examples of known anticoagulants include a thrombin inhibitor such as heparin, as well as warfarin. However, since a thrombin inhibitor acts on downstream reactions of the blood coagulation cascade and hence cannot control the consumption of coagulation factors that lead to thrombin generation upon excess inhibition of coagulation, such a thrombin inhibitor involves a problem of hemorrhage tendency in clinical use. Likewise, warfarin inhibits the production of many blood coagulation factors and also involves a problem of hemorrhage tendency in clinical use, as in the case of a thrombin inhibitor.

[0008] As mentioned above, factor VIIa is located upstream in the extrinsic pathway and hence an inhibitor against factor VIIa will not affect the intrinsic coagulation pathway. That is, such an inhibitor will be able to leave the resistance against hemorrhage. This suggests that a factor VIIa inhibitor is expected to reduce the hemorrhage tendency, a side effect of existing anticoagulants. Thus, a factor VIIa inhibitor is expected to be effective in preventing or treating pathological conditions associated with the extrinsic coagulation pathway, e.g., chronic thrombosis (more specifically, post-operative deep vein thrombosis, post-PTCA restenosis, DIC (disseminated intravascular coagulation), cardioembolic strokes, cardiac infarction and cerebral infarction).

[0009] To date, some compounds have been reported as factor VIIa inhibitors (see, e.g., WO00/41531, WO00/35886, WO99/41231, EP921116A, WO00/15658, WO00/30646, WO00/58346).

[0010] However, all of these compounds are insufficient to have an inhibitory activity against factor VIIa or a selective inhibitory activity against extrinsic blood coagulation; there is a need to develop an agent having an improved inhibitory activity or an improved selective inhibitory activity.

[0011] Recent studies on enzyme inhibitors have tended to employ computational procedures, in which a three-dimensional enzyme model based on X-ray crystal structure analysis or the like is displayed on the screen of a computer to design a candidate compound which may have an inhibitory activity or to perform computer-aided virtual screening. Factor VIIa (hereinafter also referred to as "FVIIa") has also been studied by X-ray structure analysis to determine its three-dimensional structure in free form, in complex with soluble tissue factor (this complex being hereinafter also referred to as "factor VIIa/soluble tissue factor" or "FVIIa/sTF), and in complex with a protein inhibitor (Nature, 380, 41-46, 1996; J. Mol. Biol, 285, 2089-2104, 1999; Proc Natl Acad Sci U S A., 96, 8925-8930; J Struct Biol., 127, 213-223, 1999; Nature, 404, 465-470, 2000).

[0012] However, computational virtual docking techniques result in inaccurate estimation at present (Guidebook on

Molecular Modeling Drug Design, 129-133, 1996, ACADEMIC PRESS); on the other hand, an enzyme molecule frequently undergoes an inhibitor brinding-induced conformational change called induced fit (Guidebook on Molecular Modeling Drug Design, 133-134, 1996, ACADEMIC PRESS). For computer-aided design of inhibitors, it is therefore most desirable to perform X-ray structure analysis on each inhibitor or its structurally similar inhibitor in complex with an enzyme to clarify the details of the binding mode between inhibitor and enzyme at the atomic level. In all previously reported crystals containing factor VIIa, however, irreversible inhibitors or protein inhibitors occupy the active sites of factor VIIa, which may be used as inhibitor-binding sites. Such crystals cannot be used for X-ray crystal structure analysis of a complex between factor VIIa and a low-molecular weight reversible inhibitor (e.g., having a molecular weight less than 1000). Generally, protein crystallization usually requires high purity. A problem of protease cleavage often arises in purifying such high-purity proteins (Crystallization of Nucleic Acids and Proteins, A Practical Approach, 34, 1992, IRL PRESS). In particular, a problem of self-cleavage arises in purifying and crystallizing a protease such as factor VIIa. For this reason, an irreversible inhibitor is often used in purification and crystallization because once binding occurs, the irreversible inhibitor will not be released from the protease and allows complete prevention of self-cleavage during purification and crystallization. However, in the case of a complex with a low-molecular weight reversible inhibitor, it involves technical difficulties because there is no guarantee that self-cleavage is completely prevented during crystallization. Indeed, there has been no report showing the crystallization or three-dimensional structure of a complex between factor VIIa and a low-molecular weight reversible factor VIIa inhibitor.

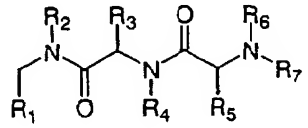
DISCLOSURE OF THE INVENTION

[0013] An object of the present invention is to provide a peptide derivative useful as a medicament, which has an inhibitory activity against blood coagulation factor VIIa or which has an excellent selective inhibitory effect on extrinsic blood coagulation.

[0014] Another object of the present invention is to provide a crystal which can be used for X-ray crystal analysis to clarify the three-dimensional structure of a complex between factor VIIa/soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, as well as a method for preparing the crystal. Yet another object of the present invention is to provide a method for designing a novel low-molecular weight reversible factor VIIa inhibitor having an excellent specific or selective inhibitory activity for factor VIIa by using three-dimensional structure information of the complex crystal, as well as a low-molecular weight reversible factor VIIa inhibitor designed by the method.

[0015] As a result of extensive and intensive efforts, the inventors of the present invention found that a peptide derivative of Formula (1) had an inhibitory activity against factor VIIa or a selective inhibitory effect on extrinsic blood coagulation, which led to the completion of the invention.

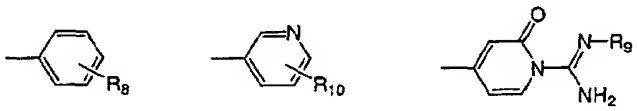
[0016] Namely, the present invention provides a compound of Formula (1):

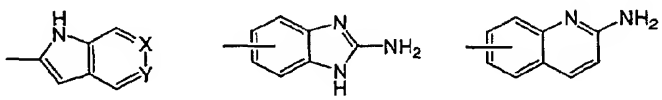


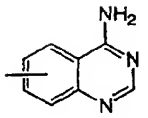
(1)

wherein

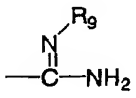
R_1 represents a group selected from the following formulae:







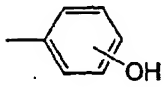
[wherein R_8 represents an amino group, an aminomethyl group or



(wherein R_9 represents a hydrogen atom, an amino group, a hydroxy group, an acyl group or an alkoxycarbonyl group having an optionally substituted linear or branched C_1-C_6 alkyl as its alkyl moiety, R_{10} represents an amino group, one of X and Y represents =CH- and the other represents =N-)];

R_2 represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group;

R_3 represents:

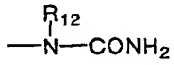


or

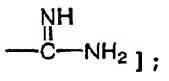
$$-(CH_2)_m-R_{11}$$

[wherein m represents an integer of 1 to 6, and R_{11} represents:

$$-CONH_2,$$



(wherein R_{12} represents a hydrogen atom or a linear or branched C_1-C_3 alkyl group) or



R_4 represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group;

R_5 represents a linear or branched C_1-C_6-alkyl group or $-CH_2-R_{13}$ (wherein R_{13} represents an optionally substituted aryl group or an optionally substituted heterocyclic group);

R_6 represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group; and

R_7 represents an optionally substituted linear or branched C_1-C_6 alkyl group or $-SO_2-R_{14}$ (wherein R_{14} represents an optionally substituted linear or branched C_1-C_8 alkyl group)

or a tautomer or enantiomer of the compound, or a hydrate or pharmaceutically acceptable salt thereof.

[0017] The present invention also provides a pharmaceutical composition comprising a compound of Formula (1).

Further, the present invention provides an antithrombotic agent comprising the compound. Furthermore, the present invention provides a blood coagulation factor VIIa inhibitor comprising the compound.

[0018] In addition, the present invention provides a crystal of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor. In one embodiment, the low-molecular weight reversible factor VIIa inhibitor is a compound of Formula (1) (wherein each symbol is as defined above).

[0019] Further, the present invention provides a method for preparing a crystal of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, which comprises the following steps (i) to (iii):

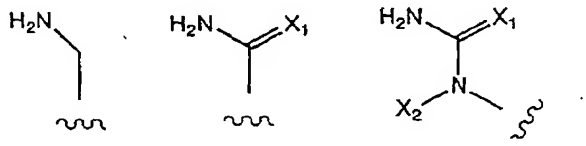
(i) preparing human factor VIIa/human soluble tissue factor, which is co-crystallizable with the low-molecular weight reversible factor VIIa inhibitor;
(ii) preparing a concentrated sample for crystallization to add the low-molecular weight reversible factor VIIa inhibitor, and
(iii) obtaining the crystal of the complex between human factor VIIa/human soluble tissue factor and the low-molecular weight reversible factor VIIa inhibitor from the concentrated sample for crystallization prepared in (ii) to add a seed crystal of a complex between a low-molecular weight irreversible or reverdible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor. In one embodiment, the low-molecular weight reversible factor VIIa inhibitor is a compound of Formula (1) (wherein each symbol is as defined above).

[0020] In addition, the present invention provides a medium carrying a part or all of structure coordinate data of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, wherein said data are obtainable by performing X-ray crystal structure analysis on the above crystal prepared for the complex between human factor VIIa/human soluble tissue factor and the low-molecular weight reversible factor VIIa inhibitor.

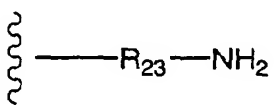
[0021] Further, the present invention provides a method for computationally designing a low-molecular weight reversible factor VIIa inhibitor using the above coordinate data. In one embodiment, the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with at least one of Asp60 side chain, Tyr94 side chain and Thr98 main chain of the human factor VIIa H chain. In another embodiment, the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with Lys192 side chain of the human factor VIIa H chain. In yet another embodiment, the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with at least one of Val170E, Gly170F, Asp170G, Ser170H, Pro170I and Gln217 of the human factor VIIa H chain. In yet another embodiment, the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with the S4 subsite of the human factor VIIa H chain through a hole extending from the S4 site to the S4 subsite.

[0022] Furthermore, the present invention provides a low-molecular weight reversible factor VIIa inhibitor designed by the above method. In one embodiment, the low-molecular weight reversible factor VIIa inhibitor comprises any one of the partial structures shown in the following Class [A-1] or [A-2] as a partial structure capable of interacting with the S2 site of human factor VIIa:

Class [A-1]:



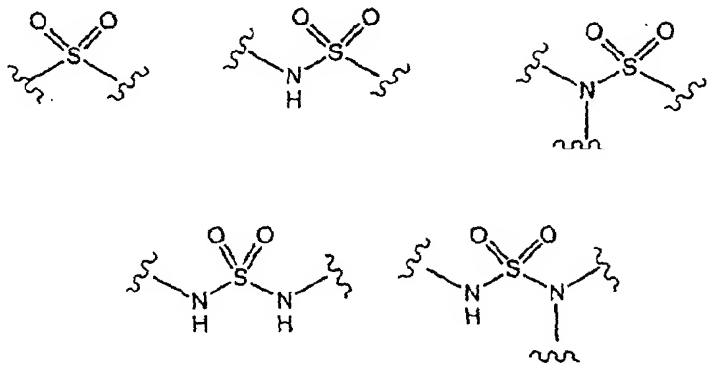
(wherein X_1 represents O or NH, and X_2 represents a hydrogen atom or a methyl group) or
Class [A-2]:



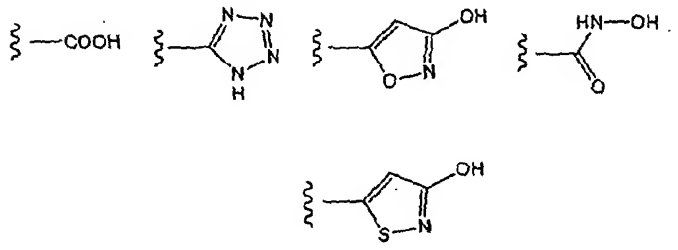
(wherein R_{23} represents a 6 or 5-membered aromatic ring containing a heteroatom(s)).

[0023] In another embodiment, the low-molecular weight reversible factor VIIa inhibitor comprises any one of the partial structures shown in the following Class [B-1], [B-2], [B-3] or [B-4] as a partial structure capable of interacting with the S1 subsite of human factor VIIa:

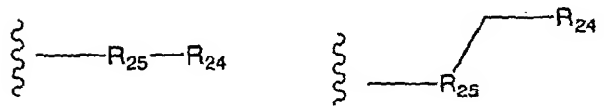
Class [B-1]:



Class [B-2]:



Class [B-3]:



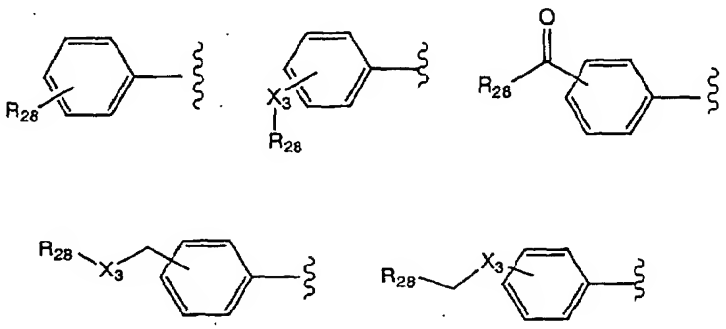
(wherein R_{24} represents the same partial structures define as Class [B-2], and R_{25} represents a 6 or 5-membered aromatic ring containing a heteroatom(s)) or

Class [B-4]:

(wherein R_{27} represents a C_1-C_3 alkylene group, R_{24} represents the same partial structures defined as Class [B-2], and R_{26} represents the same partial structures defined as Class [B-3]).

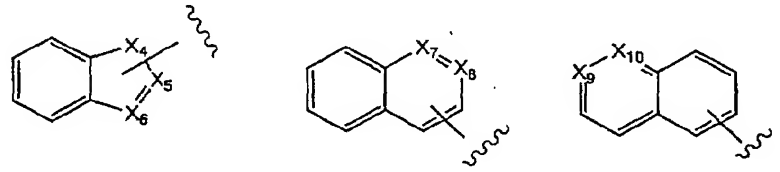
[0024] In vet another embodiment, the low-molecular weight reversible factor VIIa inhibitor comprises any one of the partial structures shown in the following Class [C-1] or [C-2] as a partial structure capable of interacting with the S4 site of human factor VIIa:

Class [C-1]:



(wherein X_3 represents O, NH or CH_2, and R_{28} represents a 6 or 5-membered aromatic ring containing a heteroatom (s)) or

Class [C-2]:



(wherein X_4 represents NH, S or O, and X_5, X_6, X_7, X_8, X_9 and X_{10} each independently represent N or CH).

[0025] In yet another embodiment, the low-molecular weight reversible factor VIIa inhibitor comprises any one of the partial structures shown in the above Class [A-1] or [A-2] as a partial structure capable of interacting with the S2 site of human factor VIIa, any one of the partial structures shown in the above Class [B-1], [B-2], [B-3] or [B-4] as a partial structure capable of interacting with the S1 subsite, and any one of the partial structures shown in the above Class [C-1] or [C-2] as a partial structure capable of interacting with the S4 site.

BRIEF DESCRIPTION OF DRAWINGS

[0026]

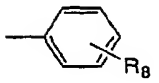
Figure 1 shows the three-dimensional conformation of the binding sites between human factor VIIa and Compound (1).

Figure 2 shows a schematic view of the binding sites between human factor VIIa and Compound (1).

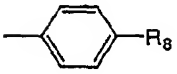
Figure 3 shows the S4 site of human factor VIIa upon binding to D-Phe-Phe-Arg-cmk (left) or Compound (1) (right)

BEST MODE FOR CARRYING OUT THE INVENTION

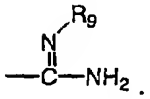
[0027] In the definition of a compound of Formula (1), the following group defined as R_1:



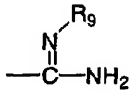
preferably has the following formula:



wherein R_8 preferably represents the following formula:

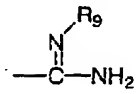


[0028] Examples of the acyl group defined as R_9 in the formula for R_8:



include alkylcarbonyl groups such as a formyl group, an acetyl group, a propionyl group, a butyryl group, an isobutyryl group, a valeryl group, an isovaleryl group, a pivaloyl group, a caproyl group and a phenylacetyl group; alkenylcarbonyl groups such as an acryloyl group, a propioloyl group, a methacryloyl group, a crotonoyl group and an isocrotonoyl group; and arylcarbonyl groups such as a benzoyl group. Preferred is an alkylcarbonyl group having a linear or branched C_1-C_6 alkyl as its alkyl moiety. Particularly preferred are an acetyl group, a propionyl group, a butyryl group, an isobutyryl group and an isovaleryl group.

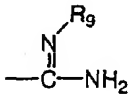
[0029] The alkoxycarbonyl group having an optionally substituted linear or branched C_1-C_6 alkyl as its alkyl moiety, defined as R_9 in the formula for R_8:



is preferably an alkoxycarbonyl group having an optionally substituted linear or branched C_1-C_4 alkyl as its alkyl moiety (wherein examples of a substituent include a phenyl group). Particularly preferred are a methoxycarbonyl group, an ethoxycarbonyl group, a t-butoxycarbonyl group and a benzyloxycarbonyl group.

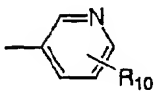
[0030] In the present invention, when expressed as "optionally substituted" or when several substitutions are possible for a given group or moiety, it is meant that the group or moiety may be substituted with one or more substituents.

[0031] R_9 in the formula for R_8:

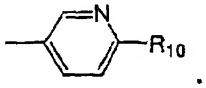


is preferably a hydrogen atom, an amino group, a hydroxy group, an acetyl group, a propionyl group, a butyryl group, an isobutyryl group, an isovaleryl group, a methoxycarbonyl group, an ethoxycarbonyl group, a t-butoxycarbonyl group or a benzyloxycarbonyl group.

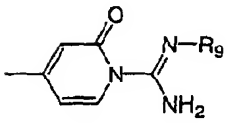
[0032] The following group defined as R_1:



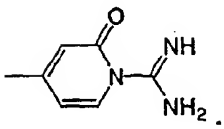
preferably has the following formula:



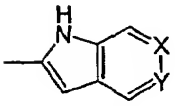
[0033] The following group defined as R_1:



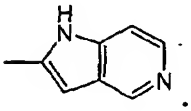
preferably has the following formula:



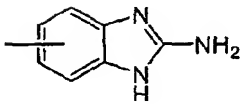
[0034] The following group defined as R_1:



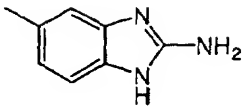
preferably has the following formula:



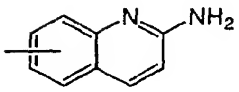
[0035] The following group defined as R_1:



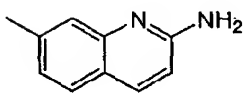
preferably has the following formula:



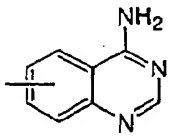
[0036] The following group defined as R_1:



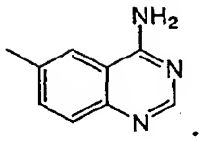
preferably has the following formula:



[0037] The following group defined as R_1:

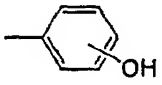


preferably has the following formula:

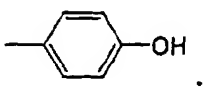


[0038] The linear or branched C_1-C_6 alkyl group defined as R_2 is preferably a linear or branched C_1-C_3 alkyl group, and particularly a methyl group.

[0039] The following group defined as R_3:

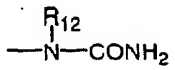


preferably has the following formula:

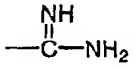


m in the group $-(CH_2)_m-R_{11}$ defined as R_3 is preferably an integer of 1 to 3, and particularly 2.

[0040] R_{11} in the group $-(CH_2)_m-R_{11}$ defined as R_3 is preferably $-CONH_2$,



or

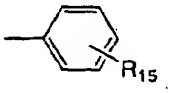


(wherein R_{12} preferably represents a hydrogen atom or a linear or branched C_1-C_3 alkyl group, and particularly represents a methyl group).

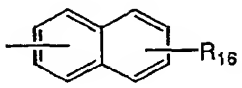
[0041] The linear or branched C_1-C_6 alkyl group defined as R_4 is preferably a linear or branched C_1-C_3 alkyl group, and particularly a methyl group.

[0042] The linear or branched C_1-C_6 alkyl group defined as R_5 is preferably a linear or branched C_1-C_4 alkyl group.

[0043] The optionally substituted aryl group as R_{13} in the group $-CH_2-R_{13}$ defined as R_5 is preferably a group of the following formula:



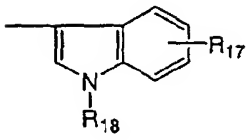
[wherein R_{15} preferably represents a hydrogen atom, an optionally substituted aryl group (wherein examples of the aryl group include a phenyl group and a naphthyl group, with a phenyl group being preferred, and examples of a substituent include a linear or branched C_1-C_3 alkoxy group, a linear or branched C_1-C_3 alkyl group which may be substituted with a halogen atom, a nitro group and an amino group), a C_1-C_3 alkyl group which may be substituted with a halogen atom, a linear or branched C_1-C_3 alkoxy group, a halogen atom, an arylcarbonyl group (wherein examples of the aryl group include a phenyl group and a naphthyl group, with a phenyl group being preferred), an alkylcarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety, a nitro group, or an amino group, and particularly represents a hydrogen atom, a t-butyl group, a methoxy group, a bromine atom, a chlorine atom, a benzoyl group, or a phenyl group which may be substituted with a methoxy group or a trifluoromethyl group or a nitro group or an amino group] or



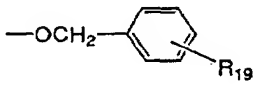
(wherein R_{16} preferably represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group, and particularly represents a hydrogen atom).

[0044] The optionally substituted heterocyclic group as R_{13} in the group $-CH_2-R_{13}$ defined as R_5 contains a 5- to 10-membered monocyclic or condensed ring having at least one nitrogen atom, oxygen atom and/or sulfur atom as a ring member. Examples include furan, thiophene, pyran, pyrrole, pyridine, indole, benzofuran, benzothiophene, benzopyran and benzothiopyran. Examples of a substituent on the optionally substituted heterocyclic group include those listed below for R_{17} and R_{18}.

[0045] The optionally substituted heterocyclic group as R_{13} in the group $-CH_2-R_{13}$ defined as R_5 is preferably a group of the following formula:



In the above formula, R_{17} preferably represents a hydrogen atom, a hydroxy group, a linear or branched C_1-C_6 alkyl group, a linear or branched C_1-C_6 alkoxy group, -O-$(CH_2)_n$-OH (wherein n represents an integer of 1 to 5), -O-$(CH_2)_p$-COOH (wherein p represents an integer of 1 to 5), -O-$(CH_2)_q$-NH_2 (wherein q represents an integer of 1 to 5),



(wherein R_{19} represents a hydrogen atom, a hydroxy group, a carboxyl group, a linear or branched C_1-C_6 alkyl group, a halogen atom, a linear or branched C_1-C_6 alkoxy group, or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety), or -OSO_2-R_{20} (wherein R_{20} represents a linear or branched C_1-C_6 alkyl group or a benzyl group).

[0046] Above all, R_{17} is preferably a hydrogen atom, a hydroxy group, a methyl group, a linear or branched C_1-C_3 alkoxy group, -O-$(CH_2)_n$-OH (wherein n represents an integer of 1 to 3), -O-$(CH_2)_p$-COOH (wherein p represents an integer of 1 to 3), -O-$(CH_2)_q$-NH_2 (wherein p represents an integer of 1 to 3), -OSO_2-R_{20} (wherein R_{20} particularly represents an ethyl group, an n-propyl group, an i-propyl group or a benzyl group), a benzyloxy group, a 3- or 4-hydroxybenzyloxy group, or a 3- or 4-carboxybenzyloxy group.

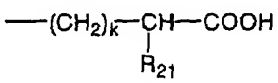
[0047] R_{18} preferably represents a hydrogen atom, a linear or branched C_1-C_6 alkyl group, a linear or branched C_1-C_6 alkylsulfonyl group, or an optionally substituted arylsulfonyl group (wherein the aryl group is preferably a phenyl group, and examples of a substituent include a linear or branched C_1-C_3 alkoxy group, a linear or branched C_1-C_3 alkyl group which may be substituted with a halogen atom, a nitro group and an amino group), and particularly represents a hydrogen atom, a methyl group, a methanesulfonyl group or a benzenesulfonyl group.

[0048] The linear or branched C_1-C_6 alkyl group defined as R_6 is preferably a linear or branched C_1-C_3 alkyl group.

[0049] Examples of a substituent on the optionally substituted linear or branched C_1-C_6 alkyl group defined as R_7 include a carboxyl group, an amino group, a mono- or di-substituted alkylamino group having a C_1-C_6 alkyl as its alkyl moiety, and an alkylcarbonylamino group having a C_1-C_6 alkyl as its alkyl moiety.

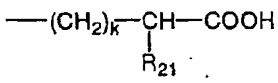
[0050] The alkyl moiety of the optionally substituted linear or branched C_1-C_6 alkyl group defined as R_7 is preferably a linear or branched C_1-C_4 alkyl group.

[0051] The optionally substituted linear or branched C_1-C_6 alkyl group defined as R_7 is preferably a linear or branched C_1-C_4 alkyl group or a group of the following formula:



[wherein k represents an integer of 0 to 3, and R_{21} represents a hydrogen atom or -NHR_{22} (wherein R_{22} represents a linear or branched C_1-C_3 alkyl group or an alkylcarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety)].

[0052] Above all, in the formula:



k is particularly an integer of 0 to 2, and R_{21} is preferably a hydrogen atom or -NHR_{22} (wherein R_{22} represents a methyl group or an acetyl group).

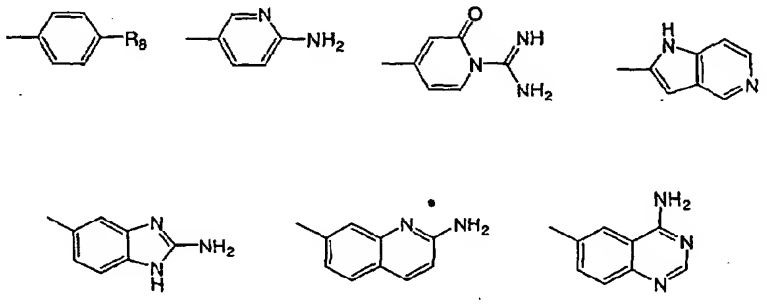
[0053] Examples of a substituent on the optionally substituted linear or branched C_1-C_8 alkyl group defined as R_{14} in the group $-SO_2-R_{14}$ defined as R_7 include (a) a carboxyl group, (b) an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety, and (c) a phenyl group which may be substituted with a carboxyl group or the like.

[0054] The alkyl moiety of the optionally substituted linear or branched C_1-C_8 alkyl group defined as R_{14} is preferably a linear or branched C_1-C_6 alkyl group.

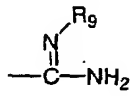
[0055] The optionally substituted linear or branched C_1-C_8 alkyl group defined as R_{14} is preferably (a) an optionally substituted linear or branched C_1-C_6 alkyl group (wherein said alkyl group may be substituted with a carboxyl group or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety), or (b) $-CH_2-R_{23}$ (wherein R_{23} represents an optionally substituted phenyl group, which may be substituted with a carboxyl group or the like).

[0056] In particular, R_{14} is preferably a benzyl group, a 2-, 3- or 4-carboxybenzyl group, or an optionally substituted linear or branched C_1-C_4 alkyl group (wherein said alkyl group may be substituted with a carboxyl group or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety).

[0057] R_1 is preferably selected from the following formulae:

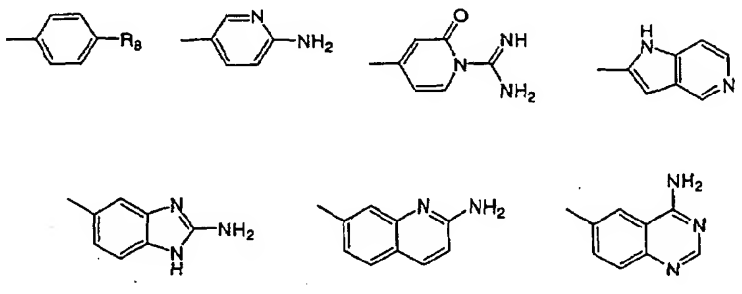


[wherein R_8 represents:

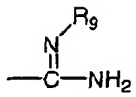


(wherein R_9 represents a hydrogen atom, an amino group, a hydroxy group, an acyl group, or an alkoxycarbonyl group having an optionally substituted linear or branched C_1-C_6 alkyl as its alkyl moiety)].

[0058] Above all, R_1 is particularly selected from the following formulae:



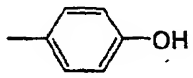
[wherein R_8 represents:



(wherein R_9 represents a hydrogen atom, an amino group, a hydroxy group, an acetyl group, a propionyl group, a butyryl group, an isobutyryl group, an isovaleryl group, a methoxycarbonyl group, an ethoxycarbonyl group, a t-butoxycarbonyl group or a benzyloxycarbonyl group)].

[0059] R_2 is preferably a hydrogen atom or a linear or branched C_1-C_3 alkyl group, and particularly a hydrogen atom or a methyl group.

[0060] R_3 is preferably a group of the following formula:

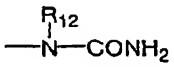


or

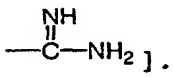
$$-(CH_2)_m-R_{11}$$

[wherein m represents an integer of 1 to 3, and R_{11} represents:

$$-CONH_2,$$

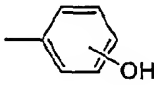


(wherein R_{12} represents a hydrogen atom or a methyl group) or



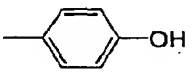
[0061] Also preferred is a compound, in which R_3 represents a linear or branched C_1-C_6 alkyl group or $-(CH_2)_m-R_{11}$ (wherein m and R_{11} are as defined above).

[0062] Also preferred is a compound, in which R_3 represents:

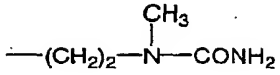


and R_7 represents $-SO_2-R_{14}$ (wherein R_{14} is as defined above).

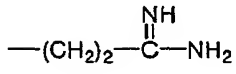
[0063] In particular, R_3 is preferably a group of the following formula:



$$-(CH_2)_2CONH_2,$$

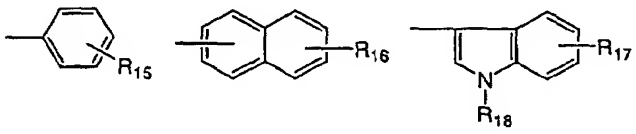


or



[0064] R_4 is preferably a hydrogen atom or a linear or branched C_1-C_3 alkyl group, and particularly a hydrogen atom or a methyl group.

[0065] R_5 is preferably a linear or branched C_1-C_6 alkyl group or $-CH_2-R_{13}$ [wherein R_{13} represents a group selected from the following formulae:

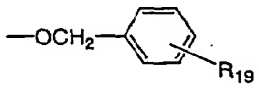


(wherein

R_{15} represents a hydrogen atom, an optionally substituted aryl group, a C_1-C_3 alkyl group which may be substituted with a halogen atom, a linear or branched C_1-C_3 alkoxy group, a halogen atom, an arylcarbonyl group, an alkylcarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety, a nitro group, or an amino group;

R_{16} represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group;

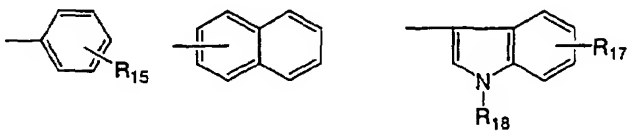
R_{17} represents a hydroxy group, a linear or branched C_1-C_6 alkyl group, a linear or branched C_1-C_6 alkoxy group, $-O-(CH_2)_n-OH$ (wherein n represents an integer of 1 to 5), $-O-(CH_2)_p-COOH$ (wherein p represents an integer of 1 to 5), $-O-(CH_2)_q-NH_2$ (wherein q represents an integer of 1 to 5),



(wherein R_{19} represents a hydrogen atom, a hydroxy group, a carboxyl group, a linear or branched C_1-C_6 alkyl group, a halogen atom, a linear or branched C_1-C_6 alkoxy group, or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety), or $-OSO_2-R_{20}$ (wherein R_{20} represents a linear or branched C_1-C_6 alkyl group or a benzyl group); and

R_{18} represents a hydrogen atom, a linear or branched C_1-C_6 alkyl group, a linear or branched C_1-C_6 alkylsulfonyl group, or an optionally substituted arylsulfonyl group)].

[0066] In particular, R_5 is preferably a linear or branched C_1-C_4 alkyl group or $-CH_2-R_{13}$ [wherein R_{13} represents a group selected from the following formulae:



(wherein

R_{15} represents a hydrogen atom, a t-butyl group, a methoxy group, a bromine atom, a chlorine atom, a benzoyl group, or a phenyl group which may be substituted with a methoxy group or a trifluoromethyl group or a nitro group or

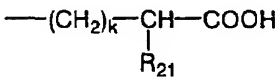
an amino group;

R_{17} represents a hydrogen atom, a hydroxy group, a methyl group, a linear or branched C_1-C_3 alkoxy group, -O-$(CH_2)_n$-OH (wherein n represents an integer of 1 to 3), -O-$(CH_2)_p$-COOH (wherein p represents an integer of 1 to 3), -O-$(CH_2)_q$-NH_2 (wherein q represents an integer of 1 to 3),-OSO_2-R_{20} (wherein R_{20} represents an ethyl group, an n-propyl group, an i-propyl group or a benzyl group), a benzyloxy group, a 3- or 4-hydroxybenzyloxy group, or a 3- or 4-carboxybenzyloxy group; and

R_{18} represents a hydrogen atom, a methyl group, a methanesulfonyl group or a benzenesulfonyl group)].

[0067] R_6 is preferably a hydrogen atom or a linear or branched C_1-C_3 alkyl group, and particularly a hydrogen atom or a methyl group.

[0068] R_7 is preferably a linear or branched C_1-C_6 alkyl group or a group of the following formula:



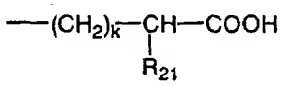
[wherein k represents an integer of 0 to 3, and R_{21} represents a hydrogen atom or -NHR_{22} (wherein R_{22} represents a linear or branched C_1-C_3 alkyl group or an alkylcarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety)] or

$$-SO_2-R_{14}$$

[wherein R_{14} represents:

(i) an optionally substituted linear or branched C_1-C_6 alkyl group (wherein said alkyl group may be substituted with a carboxyl group or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety); or
(ii) -CH_2-R_{23} (wherein R_{23} represents an optionally substituted phenyl group)].

[0069] Above all, R_7 is particularly a linear or branched C_1-C_4 alkyl group or a group of the following formula:



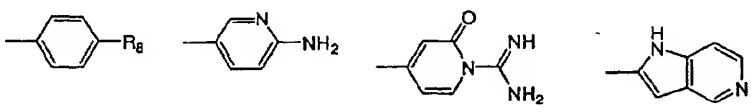
[wherein k represents an integer of 0 to 2, and R_{21} represents a hydrogen atom or -NHR_{22} (wherein R_{22} represents a methyl group or an acetyl group)] or

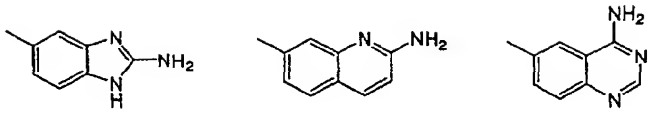
$$-SO_2-R_{14}$$

[wherein R_{14} represents a benzyl group, a 2-, 3- or 4-carboxybenzyl group, or an optionally substituted linear or branched C_1-C_4 alkyl group (wherein said alkyl group may be substituted with a carboxyl group or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety)].

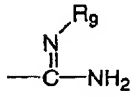
[0070] Having the definition given above for each symbol, preferred is a compound of Formula (1) wherein

R_1 is a group selected from the following formulae:





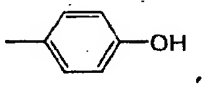
[wherein R_8 represents:

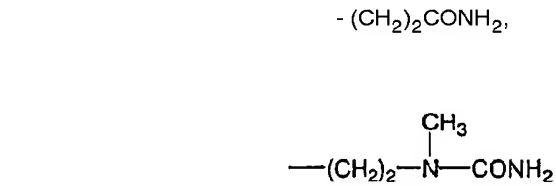


(wherein R_9 represents a hydrogen atom, an amino group, a hydroxy group, an acetyl group, a propionyl group, a butyryl group, an isobutyryl group, an isovaleryl group, a methoxycarbonyl group, an ethoxycarbonyl group, a t-butoxycarbonyl group or a benzyloxycarbonyl group)];

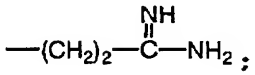
R_2 is a hydrogen atom or a methyl group;

R_3 is a group of the following formula:



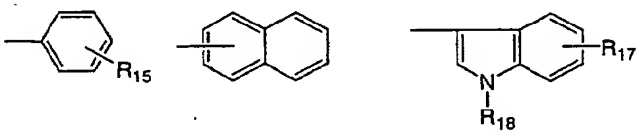


or



R_4 is a hydrogen atom or a methyl group;

R_5 is a linear or branched C_1-C_4 alkyl group or $-CH_2-R_{13}$ [wherein R_{13} represents a group selected from the following formulae:



(wherein

R_{15} represents a hydrogen atom, a t-butyl group, a methoxy group, a bromine atom, a chlorine atom, a benzoyl group, or a phenyl group which may be substituted with a methoxy group or a trifluoromethyl group or a nitro group or an amino group;

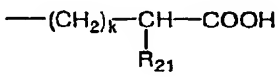
R_{17} represents a hydrogen atom, a hydroxy group, a methyl group, a linear or branched C_1-C_3 alkoxy group,

$-O-(CH_2)_n-OH$ (wherein n represents an integer of 1 to 3), $-O-(CH_2)_p-COOH$ (wherein p represents an integer of 1 to 3), $-O-(CH_2)_q-NH_2$ (wherein q represents an integer of 1 to 3), $-OSO_2-R_{20}$ (wherein R_{20} represents an ethyl group, an n-propyl group, an i-propyl group or a benzyl group), a benzyloxy group, a 3- or 4-hydroxybenzyloxy group, or a 3- or 4-carboxybenzyloxy group; and

R_{18} represents a hydrogen atom, a methyl group, a methanesulfonyl group or a benzenesulfonyl group)];

R_6 is a hydrogen atom or a methyl group; and

R_7 is a linear or branched C_1-C_4 alkyl group or a group of the following formula:

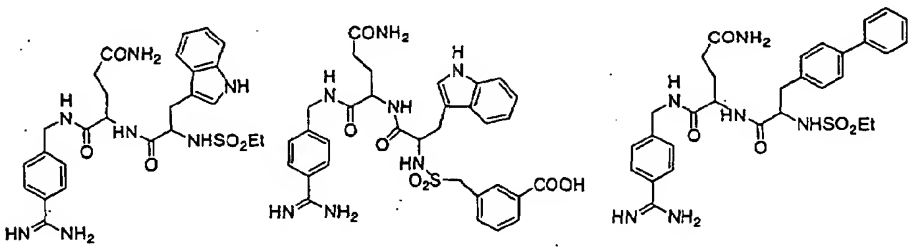


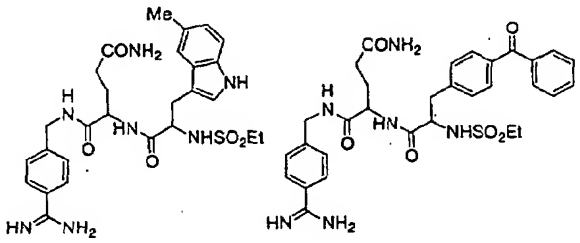
[wherein k represents an integer of 0 to 2, and R_{21} represents a hydrogen atom or $-NHR_{22}$ (wherein R_{22} represents a methyl group or an acetyl group)] or

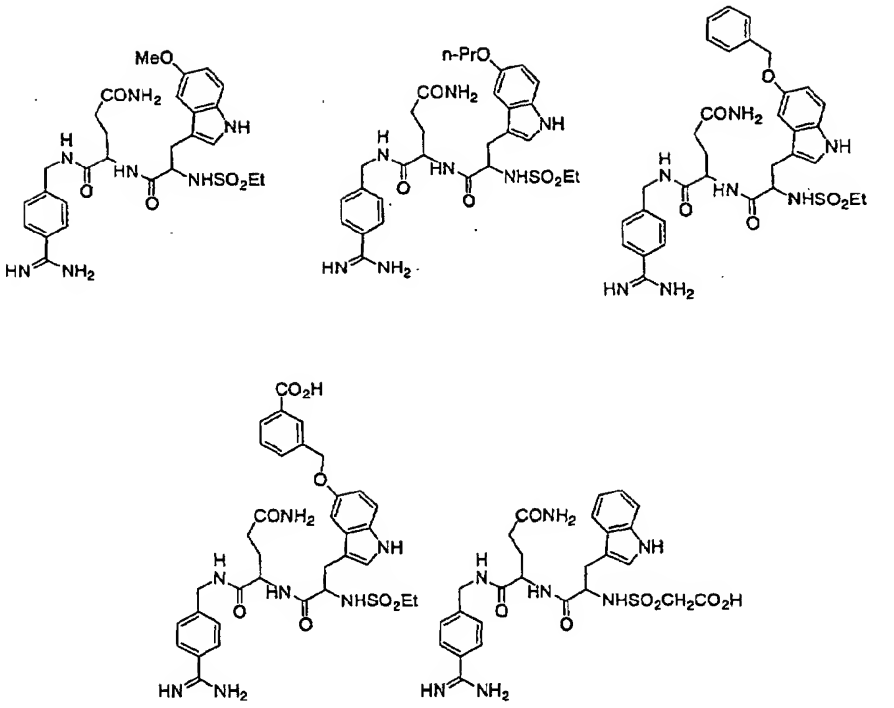
$$-SO_2-R_{14}$$

[wherein R_{14} represents a benzyl group, a 2-, 3- or 4-carboxybenzyl group, or an optionally substituted linear or branched C_1-C_4 alkyl group (wherein said alkyl group may be substituted with a carboxyl group or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety)].

Above all, particularly preferred is a compound selected from the following formulae:







[0071] Compounds of Formula (1) have enantiomers; all individual enantiomers and mixtures thereof are intended to be within the scope of the present invention. Above all, preferred are compounds having the S-configuration at the carbon atom attached to R_3 and having the R-configuration at the carbon atom attached to R_5 in Formula (1).

[0072] The compounds of the present invention may also be obtained as hydrates.

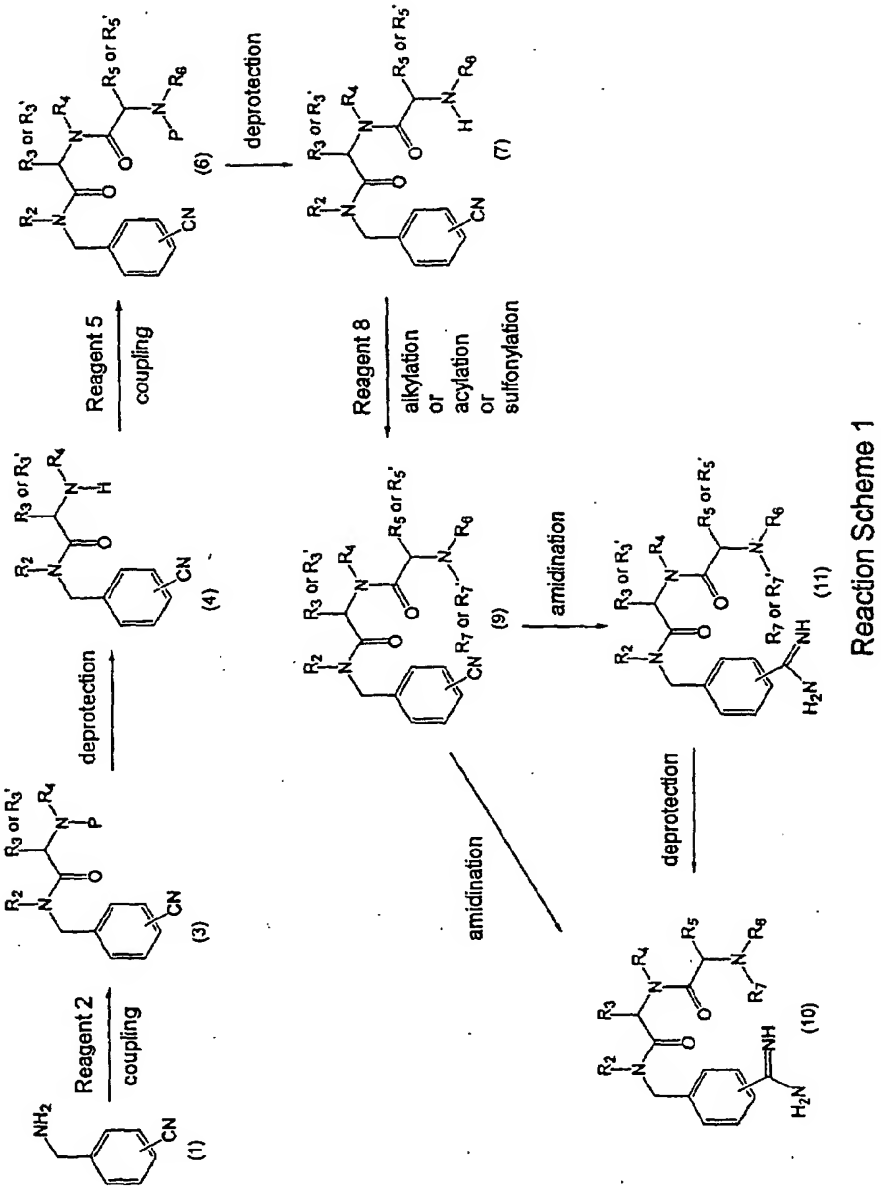
[0073] Examples of a salt-forming acid include inorganic acids such as hydrochloric acid, hydrobromic acid, hydroiodic acid, sulfuric acid and phosphoric acid, as well as organic acids such as acetic acid, oxalic acid, maleic acid, fumaric acid, citric acid, tartaric acid, methanesulfonic acid and trifluoroacetic acid.

[0074] Each compound of Formula (1) may be administered as a pharmaceutical composition in any dosage form suitable for the intended route of administration, in combination with one or more pharmaceutically acceptable diluents, wetting agents, emulsifiers, dispersants, auxiliary agents, preservatives, buffers, binders, stabilizers and the like. It may be administered parenterally or orally.

[0075] The dose of the compound can be determined as appropriate for the physique, age and physical condition of a patient, severity of the disease to be treated, elapsed time after onset of the disease, etc. For example, it is usually used at a dose of 1 to 1000 mg/day/person for oral administration and at a dose of 0.1 to 100 mg/day/person for parenteral administration (by intravenous, intramuscular or subcutaneous route).

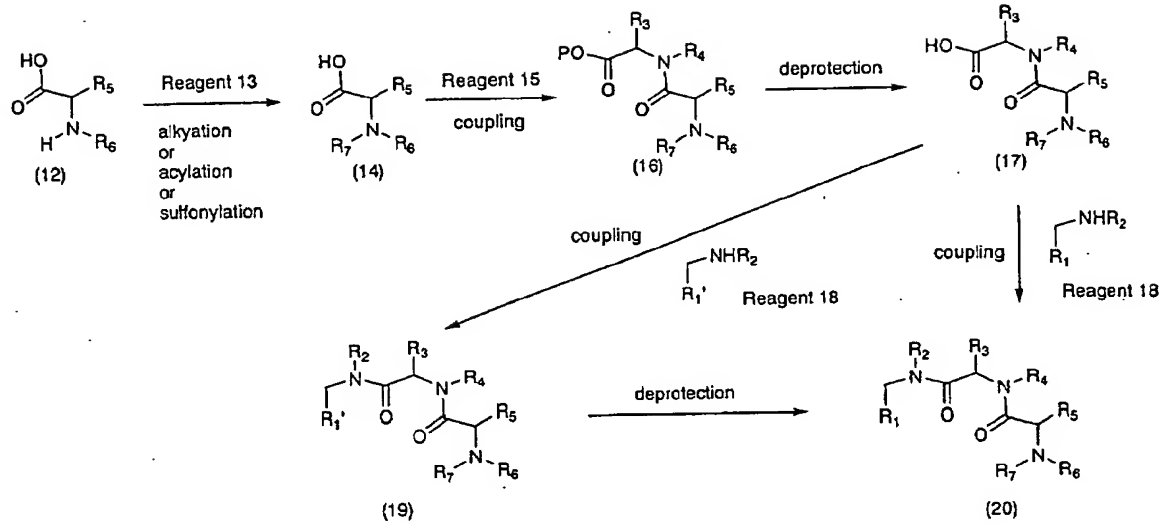
[0076] The compounds of Formula (1) can be prepared as shown in the following Reaction Schemes 1 to 6.

Reaction Scheme 1



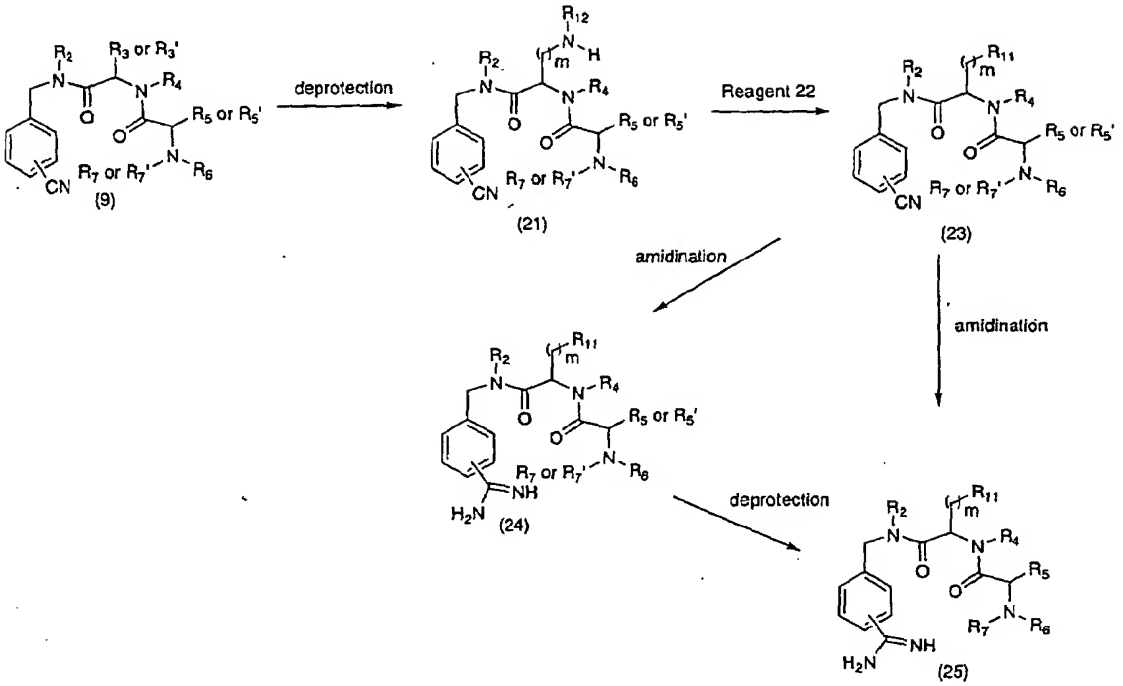
Reaction Scheme 1

Reaction Scheme 2



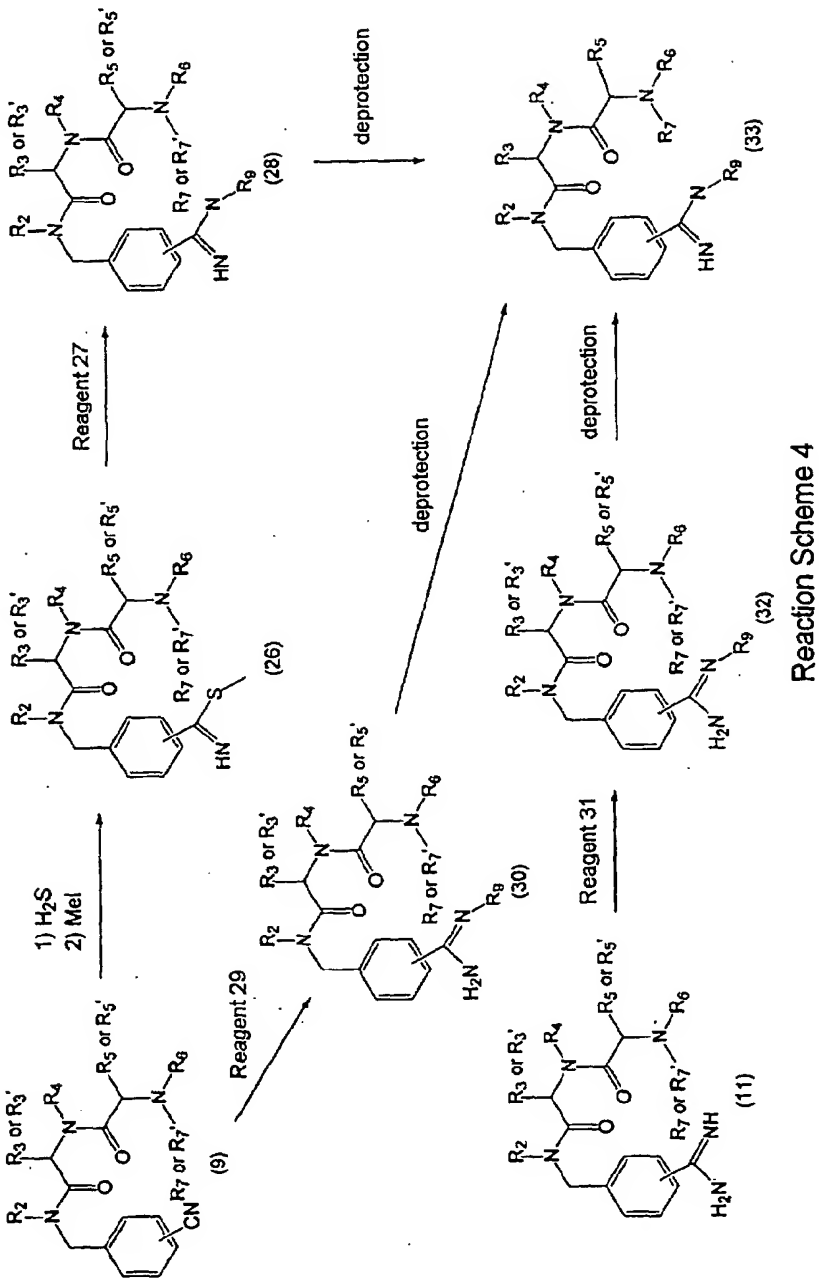
Reaction Scheme 2

Reaction Scheme 3



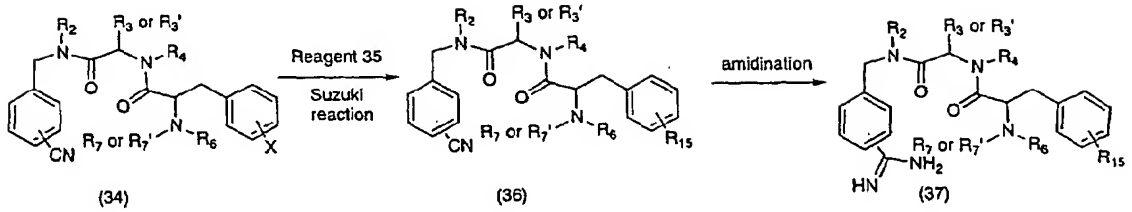
Reaction Scheme 3

Reaction Scheme 4



Reaction Scheme 4

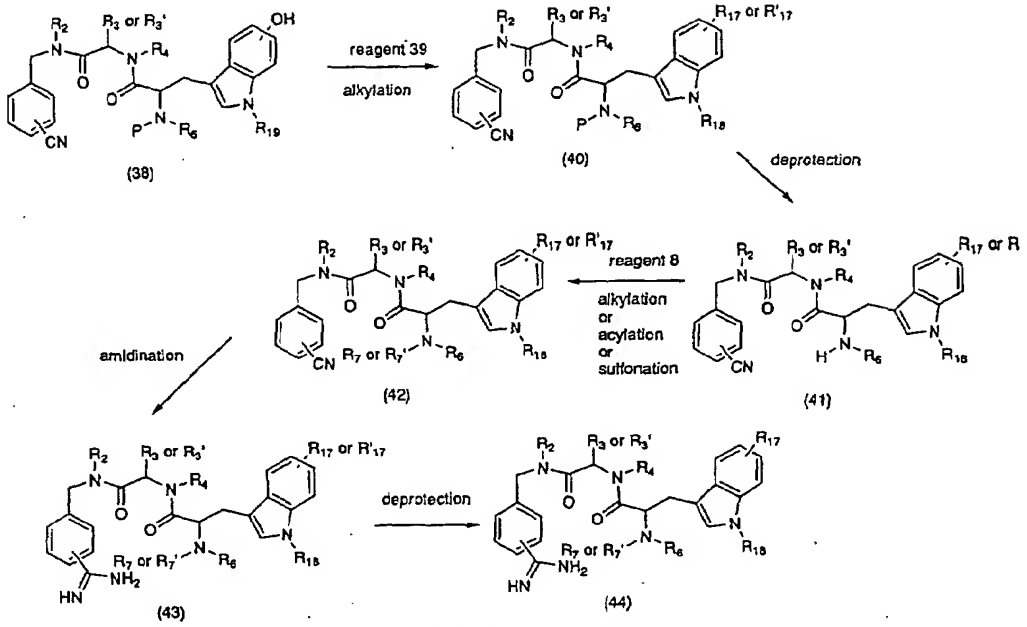
Reaction Scheme 5



Reaction Scheme 5

Reaction Scheme 6

[0077]



Reaction Scheme 6

[0078] In Reaction Schemes 1 to 6, the substituents R_1, R_2,··· and R_n are each as defined above, and R_1', R_2' ,··· and R_n' represent the respective corresponding protected forms of R_1, R_2,··· and R_n. Examples of protecting groups include those described in Principle and Experiments of Peptide Synthesis (Maruzen Co., Ltd., 1985) or PROTECTING GROUP IN ORGANIC SYNTHESIS SECOND EDITION (JOHN WILEY & SONS, INC, 1991), e.g., a t-butoxycarbonyl (Boc) group, a benzyloxycarbonyl (Cbz) group, a 9-fluorenylmethoxycarbonyl (Fmoc) group.

[0079] Likewise, P represents a commonly-used protecting group, such as those described in Principle and Experiments of Peptide Synthesis (Maruzen Co., Ltd., 1985) or PROTECTING GROUP IN ORGANIC SYNTHESIS SECOND EDITION (JOHN WILEY & SONS, INC 1991).

[0080] X represents a halogen atom such as chloride, bromide or iodide.

[0081] Starting materials in the individual reaction steps are known per se or can be prepared in a known manner.

[0082] All reactions in the individual reaction steps can be performed in a known manner.

[0083] Likewise, other starting materials and individual reagents used here are also known per se or can be prepared in a known manner.

[0084] The preparation of the compounds according to the present invention will be illustrated in more detail, in line with the above-mentioned reaction schemes.

Reaction Scheme 1

[0085] Intermediate (3) may be obtained through condensation between Starting material (1) and Reagent 2 (listed in Table A-1 to Table A-34; this reagent being commercially available or easy to synthesize by known synthesis procedures).

[0086] The condensation used here may be accomplished as described in Principle and Experiments of Peptide Synthesis (Maruzen Co., Ltd., 1985), for example, by commonly-used active ester method, acid anhydride method, azide method or acid chloride method, or using various condensing agents. Examples of a condensing agent available for use include commonly-used reagents such as those described in Peptide Synthesis Handbook (Novabiochem, 1998), e.g., N,N'-dicyclohexylcarbodiimide (DCC), water-soluble carbodiimide (WSCI), carbonyldiimidazole (CDI), diphenylphosphorylazide (DPPA), Bop reagent, Pybop reagent, 2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HBTU), 2-(1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium tetrafluoroborate (TBTU) and 2-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HATU). The reaction may be carried out in a routine manner with an appropriate solvent (e.g., dimethylformamide, dichloromethane) at room temperature or under cooling or heating conditions.

[0087] Intermediate (4) may be obtained from Intermediate (3) through appropriate amino deprotection, for example, as described in Principle and Experiments of Peptide Synthesis (Maruzen Co., Ltd., 1985). The reaction may be carried out in a routine manner with or without an appropriate solvent (e.g., dichloromethane, dimethylformamide) at room temperature or under cooling or heating conditions.

[0088] Intermediate (6) may be obtained through condensation between Intermediate (4) and Reagent 5 (listed in Table A-1 to Table A-34; this reagent being commercially available or easy to synthesize by known synthesis procedures) in the same manner as described above.

[0089] Intermediate (7) may be obtained from Intermediate (6) through amino deprotection as described above. The reaction may be carried out in a routine manner with or without an appropriate solvent (e.g., dichloromethane, dimethylformamide) at room temperature or under cooling or heating conditions.

[0090] Intermediate (9) may be obtained from Intermediate (7) through commonly-used alkylation, acylation or sulfonylation with Reagent 8 (listed in Table A-1 to Table A-34; this reagent being commercially available or easy to synthesize by known synthesis procedures). The reaction may be carried out in a routine manner with an appropriate solvent (e.g., dimethylformamide, dichloromethane) at room temperature or under cooling or heating conditions.

[0091] Compound (10) and Intermediate (11) may be derived from Intermediate (9) in a known manner as described in JP 09-509937 A, the Chemistry of Amidines and Imidates (JOHN WILEY & SONS, INC, 1991), etc.

[0092] For example, Compound (10) may be obtained by treating Intermediate (9) with a strong acid and then reacting it with an ammonium salt or ammonia. The reaction may be carried out in a routine manner with an appropriate solvent (e.g., methanol, ethanol) at room temperature or under cooling or heating conditions.

[0093] Compound (10) may also be obtained from Intermediate (11) through appropriate deprotection, for example, as described in Principle and Experiments of Peptide Synthesis (Maruzen Co., Ltd., 1985). The reaction may be carried out in a routine manner with or without an appropriate solvent (e.g., dichloromethane, dimethylformamide, water, ethanol) at room temperature or under cooling or heating conditions.

Reaction Scheme 2

[0094] Intermediate (14) may be obtained from Starting material (12) through commonly-used alkylation, acylation or sulfonylation with Reagent 13 (this reagent being an alkyl halide, an acyl chloride or sulfonyl chloride, which is commercially available or easy to synthesize by known synthesis procedures). The reaction may be carried out in a routine manner with an appropriate solvent (e.g., dimethylformamide, dichloromethane) at room temperature or under cooling or heating conditions.

[0095] Intermediate (16) may be obtained through condensation between Intermediate (14) and Reagent 15 (this

reagent being a naturally-occurring or modified amino acid, which is commercially available or easy to synthesize by known synthesis procedures) in the same manner as described above.

[0096] Intermediate (17) may be obtained from Intermediate (16) through appropriate deprotection. The reaction may be carried out in a routine manner with an appropriate solvent (e.g., water, methanol, ethanol) at room temperature or under cooling or heating conditions.

[0097] Intermediate (19) may be obtained through condensation between Intermediate (17) and Reagent 18 (listed in Table A-27; this reagent being commercially available or easy to synthesize by known synthesis procedures), while Compound (20) may be obtained through condensation between Intermediate (17) and Reagent 18 in the same manner as described above.

[0098] Compound (20) may also be obtained from Intermediate (19) through appropriate deprotection.

Reaction Scheme 3

[0099] Compound (21) may be obtained from Intermediate (9) through appropriate deprotection.

[0100] Compound (23) may be obtained through reaction between Intermediate (21) and Reagent 22 (listed in Tables A-28 to 29; this reagent being commercially available or easy to synthesize by known synthesis procedures). The reaction may be carried out in a routine manner with an appropriate solvent (e.g., dichloromethane, dimethylfonnamide, water, tetrahydrofuran) at room temperature or under cooling or heating conditions.

[0101] Intermediate (24) and Compound (25) may be obtained through amidination as described above.

[0102] Intermediate (25) may also be obtained from Intermediate (24) through appropriate deprotection.

Reaction Scheme 4

[0103] Intermediate (26) may be obtained from Intermediate (9) in a known manner, for example, according to the method of Lee, et al. (Bioorg. Med. Chem. Lett. 869-876, 6, 1998).

[0104] Intermediate (28) may be obtained from Intermediate (26) and Reagent 27 (this reagent being a compound of Formula: NH_2-R_9 (wherein R_9 is as defined above), which is commercially available or easy to synthesize by known synthesis procedures) in a known manner, for example, according to the method of Lee, et al. (Bioorg. Med. Chem. Lett. 869-876, **6**, 1998).

[0105] Intermediate (30) may be obtined from Intermediate (9) and Reagent 29 (this reagent being a compound of Formula: NH_2-R_9 (wherein R_9 is as defined above), which is commercially available or easy to synthesize by known synthesis procedures) in a known manner, for example, according to the method of Trucker, et al. (Bioorg. Med. Chem. 601-616, **8**, 2000).

[0106] Intermediate (32) may be obtained from Intermediate (11) and Reagent 31 (this reagent being an amine protecting group, such as a Boc group or a Cbz group), as described in Principle and Experiments of Peptide Synthesis (Maruzen Co., Ltd., 1985) or PROTECTING GROUP IN ORGANIC SYNTHESIS SECOND EDITION (JOHN WILEY & SONS, INC 1991). Examples of Reagent (31) include a t-butyloxycarbonyl group, a benzyloxycarbonyl group, an acetyl group and a 9-fluorenylmethyloxycarbonyl group. The reaction may be carried out in a routine manner with an appropriate solvent (e.g., dichloromethane, dimethylformamide) at room temperature or under cooling or heating conditions.

[0107] Compound (33) may be obtained from Intermediate (28), (30) or (32) through appropriate deprotection.

Reaction Scheme 5

[0108] Intermediate (34) may be obtained in the same manner as described above for Intermediate (9).

[0109] Intermediate (36) may be obtained from Intermediate (34) and Reagent 35 (listed in Tables A-30 to 31; this reagent being commercially available or easy to synthesize by known synthesis procedures) through the Suzuki reaction in the presence of a palladium catalyst, for example, according to the method of Ellman, et al. (J. Am. Chem. Soc. 11171-11172, **161**, 1994). This reaction may be carried out in a solvent commonly used for the Suzuki reaction, e.g., an ether solvent, an aromatic hydrocarbon solvent, acetonitrile, dimethylformamide, or a mixed solvent thereof with water, preferably in tetrahydrofuran, more preferably in a mixed solvent of tetrahydrofuran with water. Examples of a reagent available for use as a palladium catalyst include tetrakis(triphenylphosphine)palladium, palladium acetate, dichlorobis(benzonitrile)palladium and tris(dibenzylideneacetone)dipalladium, with tetrakis(triphenylphosphine)palladium and tris(dibenzylideneacetone)dipalladium being preferred.

[0110] Compound (37) may be obtained from Intermediate (36) through amidination as described above.

Reaction Scheme 6

[0111] Intermediate (38) may be obtained according to the above Reaction Scheme 1.

[0112] Intermediate (40) may be obtained from Intermediate (38) through commonly-used alkylation with Reagent 39 (listed in Tables A-32 to 34). The reaction may be carried out in a routine manner in the presence of an appropriate base (e.g., sodium hydride, cesium carbonate, potassium carbonate, sodium hydroxide) using an appropriate solvent (e.g., dimethylformamide, tetrahydrofuran) at room temperature or under cooling or heating conditions.

[0113] Intermediate (41) may be obtained from Intermediate (40) through deprotection as described above.

[0114] Intermediate (42) may be obtained from Intermediate (41) through alkylation, acylation or sulfonylation with Reagent 8, as described above.

[0115] Intermediate (43) may be obtained from Intermediate (42) through amidination as described above.

[0116] Compound (44) may be obtained from Intermediate (43) through appropriate deprotection.

[0117] As used herein, the term "low-molecular weight factor VIIa inhibitor" refers to an agent having an inhibitory activity against factor VIIa. This term encompasses every compound having such a property, above all, synthetic or natural low-molecular weight compounds or peptide derivatives with a molecular weight less than 1000. The inhibitory activity against factor VIIa may be determined, for example, as described below in the Test Example.

[0118] The term "irreversible factor VIIa inhibitor" refers to a factor VIIa inhibitor having a group capable of reacting with factor VIIa, which makes covalent bond with the factor VIIa. In the case of a serine protease such as factor VIIa, a chloromethylketone group may be used as a group capable of reacting with the protease to form a covalent bond with the Ser residue at the active center of the enzyme, resulting in irreversible inhibition. The term "reversible factor VIIa inhibitor" refers to a factor VIIa inhibitor whose binding to factor VIIa is not irreversible. The term "low-molecular weight reversible factor VIIa inhibitor" refers to a low-molecular weight factor VIIa inhibitor whose binding to factor VIIa is not irreversible.

[0119] To overcome the problems, the inventors of the present invention have established a method for preparing a crystal of a complex between a low-molecular weight reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor. The resulting crystal can be used for X-ray crystal structure analysis to provide accurate three-dimensional structure information about the binding mode between the low-molecular weight reversible factor VIIa inhibitor and human factor VIIa. Upon processing by a computer, this three-dimensional structure information allows a visual and numerical representation of the binding mode between the low-molecular weight reversible inhibitor and factor VIIa. This is advantageous in evaluating interactions important for binding to factor VIIa.

[0120] Starting from the structure of the complex between the low-molecular weight reversible VIIa inhibitor and factor VIIa, which is determined by X-ray structure analysis, it is further possible to design a low-molecular weight reversible inhibitor highly specific to factor VIIa by making virtual modifications to the inhibitor molecule. Such computational virtual evaluation is advantageous in facilitating the molecular design of low-molecular weight reversible inhibitors because it requires much less time than actual compound synthesis.

[0121] It is also possible to identify accurate sites allowing interactions important for the improvement of specificity to factor VIIa, upon analyzing the relationship between factor VIIa-inhibiting activity or selectivity and the binding mode between a low-molecular weight reversible VIIa inhibitor and factor VIIa. Based on the thus confirmed information about interactions important for the specificity to factor VIIa, the low-molecular weight reversible inhibitor molecule can further be modified on a computer to have interactions important for the specificity to factor VIIa in a case where the binding mode between the inhibitor molecule and factor VIIa or its structurally similar serine protease (e.g., thrombin, trypsin, factor Xa) has been identified or estimated by X-ray crystal structure analysis and/or computer modeling. Although inhibitor-enzyme interactions are very complex processes and there is a limit to accuracy in now-available computational virtual evaluation alone, more efficient molecular design can be accomplished using such interactions whose effectiveness has been confirmed experimentally.

[Crystal of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor]

[0122] This refers to a crystal composed of human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, which belongs to the orthorhombic system of space group $P2_12_12_1$ with unit cell parameters a = 71.4 Å ± 5%, b = 82.5 Å ± 5%, c = 123.3 Å ± 5% and $\alpha = \beta = \gamma = 90°$ and which contains one complex between human factor VIIa/human soluble tissue factor and the reversible factor VIIa inhibitor in the asymmetric unit.

[0123] In such a complex crystal, the low-molecular weight reversible factor VIIa inhibitor is preferably a compound of Formula (1) (wherein each symbol is as defined above).

[Method for crystallizing a complex between human factor VIIa/human soluble tissue factor and a reversible factor VIIa inhibitor]

[0124] Human factor VIIa used for crystallization may be prepared as follows. Human factor VII is expressed in cells transformed with a vector encoding human factor VII, purified by column chromatography and then converted into the active form, factor VIIa, which is further purified by column chromatography. Instead of this recombinant factor VIIa, a human FVIIa formulation (NovoSeven, Novo Nordisk Pharma Ltd.) may also be used after purification by column chromatography.

[0125] Human soluble tissue factor used for crystallization may be prepared by expression in appropriate cells or microorganism cells (particularly, *E. coli* cells) transformed with a vector encoding the extracellular domain of human tissue factor, and subsequent purification by column chromatography.

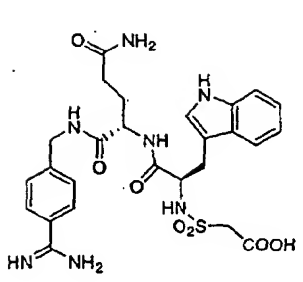
[0126] The thus prepared human factor VIIa and human soluble tissue factor may be mixed in the presence of benzamidine at an excess ratio of human soluble tissue factor to human factor VIIa, and then purified by gel filtration column chromatography with a benzamidine-free buffer to give a human factor VIIa/human soluble tissue factor complex. To this complex, a low-molecular weight reversible factor VIIa inhibitor of interest for structure analysis may be added at a concentration of around 0.5 mM or at saturation concentration (if less soluble), followed by ultrafiltration to give a concentrated sample for crystallization.

[0127] To prepare a crystal, the concentrated sample for crystallization may be subjected to vapor diffusion methods at a temperature of 25°C in a solution of 100 mM sodium cacodylate buffer (pH 5.0), 6% to 7.5% PEG4000, 5 mM $CaCl_2$ and 5% glycerol (Crystallization of Nucleic Acids and Proteins: A practical Approach, 82-90, 1992, IRL PRESS). During crystallization, it is necessary to add a seed solution prepared by crushing and diluting a crystal of a complex between a low-molecular weight irreversible or reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor in 100 mM sodium cacodylate buffer (pH 5.0), 9% PEG4000 and 5 mM $CaCl_2$ using a homogenizer. About a month later, long rod crystals (maximum size: about 1.0 mm long × 0.05 mm diameter) may be obtained for a complex between the low-molecular weight reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor. Crystallization procedures and solution conditions are not limited to those described above only. For example, crystallization may also be accomplished by static batch methods, free interface diffusion methods or dialysis methods, in addition to vapor diffusion methods.

[0128] In such a crystallization method, the low-molecular weight reversible factor VIIa inhibitor is preferably a compound of Formula (1) (wherein each symbol is as defined above).

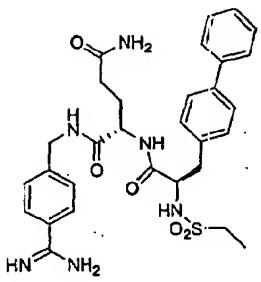
[Medium carrying a part or all of structure coordinate data of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor]

[0129] The coordinates of a complex between a low-molecular weight reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor may be obtained by revealing the three-dimensional structure of this complex crystal using X-ray crystal structure analysis, one of the three-dimensional structure determination techniques. In this technique, a crystal is irradiated with monochromatized X-ray beams to collect the intensity data of diffraction spots, based on which the electron density in the crystal unit is calculated to determine the positions of individual atoms. The three-dimensional positions of individual atoms and a variable parameter representing atomic thermal vibration called the temperature factor are refined to minimize the difference between calculated (Fc) and observed (Fo) diffraction intensity data, thereby giving the final coordinate data of the crystal structure. By way of illustration, the above-mentioned procedures is applied to the following compounds disclosed herein as examples for a low-molecular weight reversible factor VIIa inhibitor to prepare crystals of their respective complexes with factor VIIa/human soluble tissue factor, followed by X-ray crystal structure analysis to clarify their binding modes with factor VIIa.



(1)

Example 146



(2)

Example 65

[0130] Table 36 shows the coordinate data of a complex between Compound (1) and human factor VIIa/human soluble tissue factor, given in PDB format commonly used in the art for recording three-dimensional coordinates of proteins. In Table 36, the first line denotes the lattice type and symmetry of the crystal. The second and subsequent lines contain the structure coordinate data, including, from the left, atomic number, atom name, amino acid residue name, chain ID, amino acid residue number, X, Y, Z, occupancy, temperature factor, segment ID (equal to chain ID in this case) and atom type. The unit of coordinates is in Å. Amino acid residues are numbered on the basis of the residue number of the corresponding chymotrypsin amino acid residue, as described in Nature, vol. 380, pages 41-46, 1996. Factor VIIa are composed of two polypeptide chains: the longer one is herein referred to as the H chain and the shorter one as the L chain. In Table 36, chain ID indicates the following: H: factor VIIa H chain; L: factor VIIa L chain; T: soluble tissue factor; C: calcium ion; W: water molecule or I: low-molecular weight reversible factor VIIa inhibitor.

[0131] In the present invention, a part of coordinate data is intended to mean partial data of structure coordinates obtained by X-ray crystal structure analysis, particularly the coordinate data covering a low-molecular weight reversible factor VIIa inhibitor and its surrounding residues, expressed in three-dimensional form. Likewise, Table 37 shows the coordinate data of a complex between Compound (2) and human factor VIIa/human soluble tissue factor, obtained by X-ray crystal structure analysis. The coordinate data shown in Table 37 is given in PDB format for residues located exclusively within 10 Å of Compound (2).

[0132] A medium containing a part or all of coordinate data is intended to mean a computer memory or any disk device carrying a part or all of coordinate data in PDB format or equivalent information.

[Method for computationally designing a novel low-molecular weight reversible factor VIIa inhibitor using the analyzed coordinate data]

[0133] There are many computer programs for representing the three-dimensional structure of molecules such as proteins. When these software programs are combined with the structure coordinates obtained by X-ray crystal structure analysis, it is possible to make computer-aided visual representation of the structure of a complex between a low-molecular weight reversible VIIa inhibitor and human factor VIIa/human soluble tissue factor, particularly the structure surrounding the low-molecular weight reversible factor VIIa inhibitor. This allows visual recognition of interactions between the low-molecular weight reversible factor VIIa inhibitor and human FVIIa. Figure 1 shows a three-dimensional view of Compound (1) bound to active site pockets of human factor VIIa. The peptide compound of the present invention including Compound (1) will bind to human factor VIIa at 4 sites, which are designated as S1 site, S2 site, S4 site and S1 subsite, respectively. Each active site pocket is composed of amino acid residues from the human factor VIIa H chain. Hereinafter, it is not specifically noted that amino acid residues constituting active sites are found in H chain. Figure 2 shows a schematic view of the binding mode, along with main amino acid residues of human factor VIIa used for constituting the individual sites. The peptide compound including Compound (1) will bind to these residues via hydrogen bonding, ionic bonding, as well as van der Waals interaction. As used herein, the term "hydrogen bonding" refers to an electric dipole-electric dipole interaction in the form of X-H...Y, established by sandwiching hydrogen between a X-H group (wherein X represents an electronegative group) and other electronegative group Y having an unshared electron pair. This term also encompasses an interaction between ion and dipole, one of which is positively or negatively charged at physiological pH. Typically, such an interaction occurs when X and Y are N or O. The term "ionic bonding" refers to an electrostatic interaction established between a group negatively charged at physiological pH (e.g., carboxylic acid) and a group positively charged at physiological pH (e.g., amidino or amine). The term "van der Waals interaction" refers to an interaction between any atoms, which serves as a weak attraction at an appropriate

distance apart, whereas it serves as a strong repulsion at a distance less than a threshold. Every atomic species has a value called the van der Waals radius. The strongest attraction is established when a distance between two atoms is the sum of their van der Waals radii.

[0134] In these software programs, it is also possible to make virtual modification of the structure of an inhibitor molecule and to make a rough energy estimation for the influence of the modified inhibitor molecule on its binding by calculating a value called the molecular force field energy. Starting from the structure coordinates determined by X-ray crystal structure analysis, it is further possible to design a novel inhibitor capable of establishing a stronger binding to human factor VIIa by making virtual modification of the inhibitor using such programs. Such strategy is advantageous in designing low-molecular weight reversible inhibitors specific to factor VIIa because it requires much less time for evaluation than actual compound synthesis. Examples of such computer programs include, but are not limited to, QUANTA, InsightII, CHARMM, Discover and Ludi (Accelrys Inc) as well as Sybyl (Tripos Inc).

[0135] In this way, virtual modifications and evaluations can be made on inhibitors using three-dimensional structure information. However, inhibitor-enzyme binding is a very complex process and there is a limit to accuracy in now-available virtual evaluation. For this reason, a plurality of low-molecular weight reversible factor VIIa inhibitors may be analyzed for the relationship between their factor VIIa-inhibiting activity or selectivity and their binding modes determined by X-ray crystal structure analysis in order to identify sites and interactions important for binding and specificity to human factor VIIa. The thus identified sites and interactions will in turn allow computer-aided design of a low-molecular weight reversible inhibitor specific to human factor VIIa. In this way, a problem of accuracy in computational virtual evaluation of the binding activity can be overcome using such experimentally confirmed information on binding modes.

[0136] Table 41 shows the hydrogen bonding between Compound (1) and S2 site of human factor VIIa. Compound (1) has an amide group at a position where it binds to the S2 site, through which hydrogen bonds are formed between its amino moiety and the side chain carboxylic acid of Asp60, the side chain hydroxy group of Tyr94 and the main chain carbonyl oxygen of Thr98. In addition, data in Table 38 indicate that the selectivity against thrombin is higher in low-molecular weight reversible factor VIIa inhibitors capable of hydrogen bonding with these amino acid residues at the S2 site than in factor VIIa inhibitors incapable of hydrogen bonding. These findings suggest that the establishment of such hydrogen bonding is advantageous in providing the specificity to human factor VIIa. Since Asp60 is negatively charged at physiological pH, the establishment of ionic bonding is also advantageous in providing the specificity to factor VIIa.

[0137] In view of the foregoing, efficient design can be achieved for an inhibitor highly specific to human factor VIIa by modifying the inhibitor structure to include a hydrogen-bearing nitrogen atom (e.g., an amide group, an amidino group, a guanidino group, aniline, amine) or a hydrogen-bearing oxygen atom (e.g., a hydroxy group) at a position capable of hydrogen bonding or ionic bonding with all or some of the side chain carboxylic acid of Asp60, the side chain hydroxy group of Tyr94 and the main chain carbonyl oxygen of Thr98, particularly with the side chain of Asp60. The molecular design may be accomplished such that a hydrogen-bondable atom of the introduced substituent is located at a distance of 2.5 to 3.5 Å from at least one of the side chain oxygen atom of Asp60, the side chain oxygen atom of Tyr94 and the main chain oxygen atom of Thr98. Likewise, an ionic bond may be introduced such that a positively-charged atom of the introduced substituent is located at a distance of 2.5 to 4.5 Å from the side chain oxygen atom of Asp60. Alternatively, after a structure coordinate of a complex between a molecule to be modified and factor VIIa or its structurally similar protease (e.g., thrombin, trypsin, factor Xa) by modeling or X-ray crystal structure analysis is fitted to the factor VIIa part of the structure coordinates of the complex between Compound (1) or (2) and human factor VIIa/human soluble tissue factor, it may allow to introduce a substituent, which has the atoms capable of hydrogen bonding at the overlap position of the amide group of Compound (1) or (2), into the molecule to be modified.

[0138] Tables 42 and 43 show the hydrogen and/or ionic bonding between Compound (1) or (2) and S1 subsite of human factor VIIa, respectively. Each of these inhibitors has a sulfonamide group and/or carboxylic acid at a position where it binds to the S1 subsite, through which a hydrogen or ionic bond is formed with the side chain amine group of Lys192. In addition, data in Table 39 indicate that higher selectivity against thrombin is given by factor VIIa inhibitors capable of hydrogen or ionic bonding with these amino acid residues at the S1 subsite, particularly by those having carboxylic acid. These findings suggest that the establishment of such hydrogen or ionic bonding is advantageous in providing the specificity to human factor VIIa.

[0139] In view of the foregoing, efficient design can be achieved for an inhibitor highly specific to human factor VIIa by modifying the inhibitor structure to include carboxylic acid or a biological equivalent thereof (e.g., sulfonic acid, sulfonamide, sulfonurea, tetrazole) at a position capable of hydrogen or ionic bonding with the side chain amino group of Lys192. The molecular design may be accomplished such that a hydrogen-bondable atom of the introduced substituent is located at a distance of 2.5 to 3.5 Å from the side chain nitrogen atom of Lys192. Likewise, an ionic bond may be introduced such that a negatively-charged atom of the introduced substituent is located at a distance of 2.5 to 4.5 Å from the side chain nitrogen atom of Lys192. Alternatively, after a structure coordinate of a complex between a molecule to be modified and factor VIIa or its structurally similar protease (e.g., thrombin, trypsin, factor Xa) by modeling

or X-ray crystal structure analysis is fitted to the factor VIIa part of the structure coordinates of the complex between Compound (1) or (2) and human factor VIIa/human soluble tissue factor, it may allow to introduce a substituent, which has the atoms capable of hydrogen or ionic bonding at the overlap position of the sulfonamide group of Compound (2) or the carboxylic acid moiety of Compound (1), into the molecule to be modified. Since the position of Lys192 will vary depending on the structure of a compound bound thereto, the molecule may also be modified to establish hydrogen or ionic bonding with each position of Lys 192 when the Compound (1) or the Compound (2) is bounded. Furthermore, taking into account the flexibility of Lys192, the above strategy may also be applied to the structure adjusted to ensure a stable position of the Lys192 side chain in light of molecular force field energy.

[0140] Tables 44 and 45 show the van der Waals interaction between Compound (1) or (2) and S4 site of human factor VIIa, respectively. These compounds establish van der Waals interactions and hydrophobic interactions with the Trp215 side chain, the Gly216 main chain, the Gln217 side chain, the Val170E side chain, the Glyl70F main chain, the Asp170G main chain, the Ser170H main and side chains, as well as the Pro170I side chain, among amino acid residues constituting the S4 site. In addition, data in Table 40 indicate that the selectivity against thrombin is higher in Compounds (1) and (2) than in compounds modified to have a smaller area for interactions with these amino acid residues. These findings suggest that the establishment of van der Waals and hydrophobic interactions with these amino acid residues, particularly with Val170E, Gly170F, Asp170G, Ser170H, Pro170I and Gln217, is advantageous in providing the specificity to human factor VIIa. As used herein, the term "hydrophobic interaction" refers to a phenomenon in which nonpolar groups (e.g., an alkyl group, a benzene ring) are associated in water. Water molecules surrounding such nonpolar groups are in low-entropy state and hence energetically unstable. For this reason, the nonpolar groups are associated and interacted with each other to give a smaller surface area in contact with water.

[0141] In view of the foregoing, efficient design can be achieved for an inhibitor highly specific to human factor VIIa by modifying the inhibitor structure to include a more hydrophobic group (e.g., a Bi-Phe group, a naphthyl group, an indole group) at a position capable of van der Waals and hydrophobic interactions with these amino acid residues. The molecular design may be accomplished such that atoms in the introduced substituent are located at a distance of 3.5 to 4.2 Å from atoms in these amino acid residues. Alternatively, after a structure coordinate of a complex between a molecule to be modified and factor VIIa or its structurally similar protease (e.g., thrombin, trypsin, factor Xa) by modeling or X-ray crystal structure analysis is fitted to the factor VIIa part of the structure coordinates of the complex between Compound (1) or (2) and human factor VIIa/human soluble tissue factor, it may allow to introduce a substituent, which has the hydrophobic atoms at the overlap position of the indole moiety of Compound (1) or the biphenyl moiety of Compound (2), into the molecule to be modified.

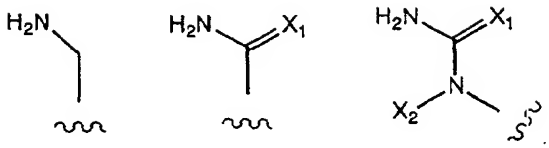
[0142] Figure 3 shows the molecular surface of the S4 site in factor VIIa upon binding to D-Phe-Phe-Arg chloromethylketone (Nature, 380, 41-46, 1996, PDB = 1DAN) or Compound (1). Upon binding to Compound (1), there appears a hole extendable to a space under the S4 site, which is not observed upon binding to D-Phe-Phe-Arg chloromethylketone. There has been no report showing such a hole or a compound resulting in such a hole. This behavior is caused by a change in the position of the Gln217 side chain when the indole ring of Compound (1) binds to a specific position in the S4 site. Under this hole, there is a space surrounded by the Cys168 side chain, the Ser170B side chain, the Ile176 side chain, the Cys182 side chain, the Trp 215 side chain, the Gly 216 main chain, the Gln 217 main and side chains, the His 224 main and side chains, the Phe225 main and side chains, the Gly 226 main chain, as well as the Val227 side chain. This space is hereinafter referred to as S4 subsite. By allowing a substituent to protrude through this hole, it is possible to establish hydrogen bonding, van der Waals interactions and hydrophobic interactions with these S4 subsite residues. When a comparison of three-dimensional structure is made with known blood coagulation-related serine proteases including thrombin, none of these proteases has a space corresponding to the S4 subsite; the establishment of interactions with the S4 subsite is advantageous in providing the specificity to human factor VIIa. For example, in a case where Compound (1) is used as an initial model for molecular design, a substituent introduced at the 5-position of the indole moiety may be allowed to protrude through this hole toward the direction of the S4 subsite.

[0143] In view of the foregoing, the compound structure can be modified to include a hydrophobic group (e.g., a benzene ring) at the position corresponding to the indole ring of Compound (1), thereby resulting in a hole extending to the S4 subsite. In addition, a substituent may be introduced in such a way as to protrude through this hole to establish hydrogen bonding, van der Waals interaction and hydrophobic interaction with the S4 subsite. These allow the design of an inhibitor highly specific to human factor VIIa.

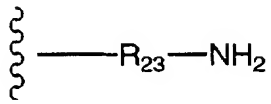
[0144] In summary, a preferred low-molecular weight reversible factor VIIa inhibitor will interact with at least one of the S2 site, S1 subsite, S4 site and S4 subsite of human factor VIIa. More specifically, a preferred low-molecular weight reversible factor VIIa inhibitor comprises at least one of the partial structures shown in the following Class [A-1], [A-2], [B-1], [B-2], [B-3], [B-4], [C-1] or [C-2].

(A) The partial structures shown in the following Class [A-1] or [A-2] are preferred for interaction with the S2 site:

Class [A-1]:



(wherein X_1 represents O or NH, and X_2 represents a hydrogen atom or a methyl group) or Class [A-2]:

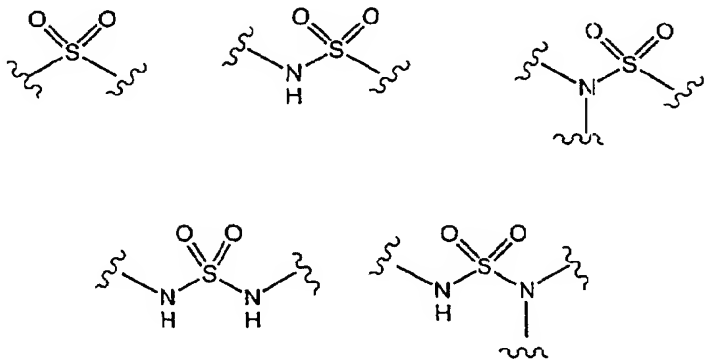


(wherein R_{23} represents a 6 or 5-membered aromatic ring containing a heteroatom(s)).

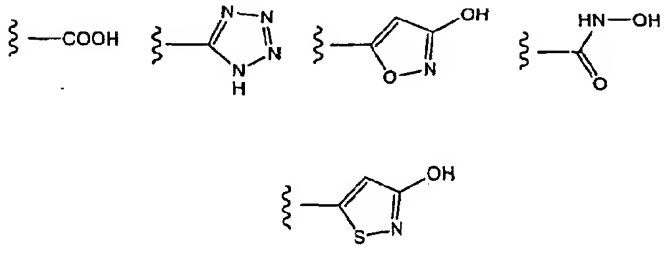
In Class [A-2], particularly preferred is a partial structure wherein R_{23} is a benzene ring, a pyridine ring or an imidazole ring.

(B) The partial structures shown in the following Class [B-1], [B-2], [B-3] or [B-4] are preferred for interaction with the S1 subsite:

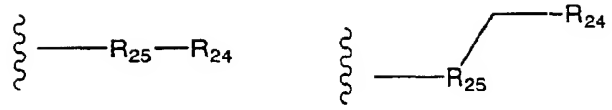
Class [B-1]:



Class [B-2]:



Class [B-3]:

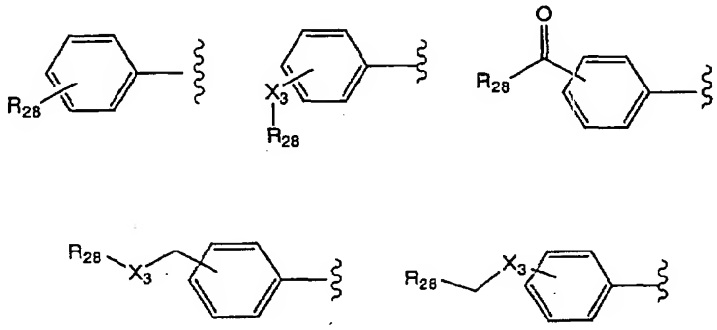


(wherein R_{24} represents the same partial structures defined as Class [B-2], and R_{25} represents a 6 or 5-membered aromatic ring containing a heteroatom(s), preferably represents a benzene ring) or
Class [B-4]:

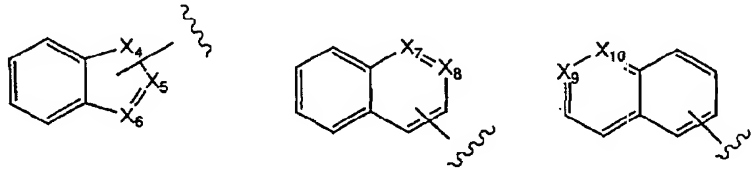
(wherein R_{27} represents a C_1-C_3 alkylene group, R_{24} represents the same partial structures defined as Class [B-2], and R_{26} represents the same partial structures defined as Class [B-3]).

(C) The partial structures shown in the following Class [C-1] or [C-2] are preferred for interaction with the S4 site:

Class [C-1]:



(wherein X_3 represents O, NH or CH_2, and R_{28} represents a 6 or 5-membered aromatic ring containing a heteroatom(s)
Class [C-2]:



(wherein X_4 represents NH, S or O, and X_5, X_6, X_7, X_8, X_9 and X_{10} each independently represent N or CH).

[0145] In Class [C-1], preferred are partial structures wherein R_{28} is a benzene ring.

[0146] More specifically, a preferred low-molecular weight reversible factor VIIa inhibitor comprises: (1) any one of the partial structures shown in the above Class [A-1] or [A-2] as a partial structure capable of interacting with the S2 site as well as any one of the partial structures shown in the above Class [B-1], [B-2], [B-3] or [B-4] as a partial structure capable of interacting with the S1 subsite; (2) any one of the partial structures shown in the above Class [A-1] or [A-2] as a partial structure capable of interacting with the S2 site as well as any one of the partial structures shown in the

above Class [C-1] or [C-2] as a partial structure capable of interacting with the S4 site; or (3) any one of the partial structures shown in the above Class [B-1], [B-2], [B-3] or [B-4] as a partial structure capable of interacting with the S1 subsite as well as any one of the partial structures shown in the above Class [C-1] or [C-2] as a partial structure capable of interacting with the S4 site.

[0147] A particularly preferred low-molecular weight reversible factor VIIa inhibitor comprises any one of the partial structures shown in the above Class [A-1] or [A-2] as a partial structure capable of interacting with the S2 site, any one of the partial structures shown in the above Class [B-1], [B-2], [B-3] or [B-4] as a partial structure capable of interacting with the S1 subsite, and any one of the partial structures shown in the above Class [C-1] or [C-2] as a partial structure capable of interacting with the S4 site.

EXAMPLES

[0148] The present invention will be further described in the following Examples, which are not intended to limit the scope of the invention. To explain the utility of the compounds according to the present invention, some representative compounds are tested for their biological activities including FVIIa-inhibiting activity in the Test Example.

[0149] In the following Examples, conventional abbreviations are used, as shown below:

DMF = N,N-dimethylformamide;
HOBt = 1-hydroxybenzotriazole;
EDC HCl = 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride;
Boc = tertiary-butoxycarbonyl;
Ac = acetyl;
Fmoc = 9-fluorenylmethoxycarbonyl; and
HPLC = high performance liquid chromatography.

[0150] NMR found in the physical property data refers to a nuclear magnetic resonance spectrum. The results are expressed as δ (delta) values in units of ppm, which are commonly used to represent chemical shifts. The measurement was carried out in the presence or absence of an internal standard (TMS; tetramethylsilane). Numerals in parentheses found next to the δ values indicate the number of hydrogen atoms, followed by the symbols s, d, t, q, m and br which represent singlet, doublet, triplet, quartet, multiplet and a broad absorption peak, respectively. Likewise, *J* represents a coupling constant.

[0151] MS refers to mass spectrometry. FAB and ESI are abbreviations for ionization techniques, Fast-Atom Bombardment Ionization and ElectroSpray Ionization, respectively.

Example 1

N^1-4-Cyanobenzyl-N^2-*t*-butoxycarbonyl-L-glutamide

[0152] To a solution of 4-cyanobenzylamine (1.6 g, 12.2 mmol) in DMF (20 ml), *t*-butoxycarbonyl-L-glutamine (2.0 g, 8.1 mmol), HOBt (1.4 g, 8.9 mmol) and EDC HCl (1.7 g, 8.9 mmol) were added and stirred at room temperature under a nitrogen stream. After 12 hours, water was added to the reaction mixture, which was then extracted with ethyl acetate. The ethyl acetate layer was washed sequentially with 10% aqueous citric acid, saturated aqueous sodium bicarbonate and saturated brine, and then dried over anhydrous magnesium sulfate. Magnesium sulfate was filtered off and the filtrate was concentrated under reduced pressure to give N^1-4-cyanobenzyl-N^2-*t*-butoxycarbonyl-L-glutamide (2.9 g, 8.1 mmol; yield 100%).
H-NMR ($CDCl_3$) δ: 1.42 (9H, s), 1.87-2.55 (4H, m), 4.14-4.27 (1H, m), 4.49 (2H, d, *J*=6 Hz), 5.47-6.02 (2H, m), 7.38 (2H, d, *J*=8 Hz), 7.60 (2H, d, *J*=8 Hz)

Example 2

N^1- 4-Cyanobenzyl-L-glutamide

[0153] To N^1-4-cyanobenzyl-N^2-*t*-butoxycarbonyl-L-glutamide (2.9 g, 8.1 mmol), a 4N hydrochloric acid/ethyl acetate solution (20 ml) was added and stirred at room temperature under a nitrogen stream. After 1 hour, the solvent was distilled off under reduced pressure and the residue was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane:methanol = 1:1) to give N^1-4-cyanobenzyl-L-glutamide (2.1 g, 8.1 mmol; yield 100%).
H-NMR (CD_3OD) δ: 1.77-2.12 (2H, m), 2.32 (3H, t, *J*=7 Hz), 3.29-3.45 (4H, m), 4.49 (2H, s), 7.50 (2H, d, *J*=8 Hz), 7.71 (2H, d, *J*=8 Hz)

Example 3

1-(*t*-Butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide

[0154] To a solution of N^1-4-cyanobenzyl-L-glutamide (300 mg, 1.2 mmol) and N-(9-fluorenylmethoxycarbonyl)-1-(*t*-butoxycarbonyl)-D-tryptophan (606 mg, 1.2 mmol) in DMF (5 ml), HOBt (176 mg, 1.2 mmol) and EDC HCl (221 mg, 1.2 mmol) were added and stirred at room temperature under a nitrogen stream. After 12 hours, water was added to the reaction mixture to precipitate N-(9-fluorenylmethoxycarbonyl)-1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide, which was then collected by filtration, washed with water and dried. The resulting N-(9-fluorenylmethoxycarbonyl)-1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide was dissolved in dichloromethane (40 ml), to which piperidine (10 ml) was then added and stirred at room temperature under a nitrogen stream. After 5 minutes, the solvent was distilled off under reduced pressure and the residue was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane:methanol = 1:0, 10:1) to give 1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (650 mg, 1.2 mmol; yield 100%).
H-NMR ($CDCl_3$) δ: 1.67 (9H, s), 1.80-2.49 (4H, m), 3.13-3.33 (2H, m), 3.70-3.79 (1H, dd, *J*=4, 9 Hz), 4.40 (2H, d, *J*=6 Hz), 4.39-4.55 (1H, m), 5.62 (1H, brs), 6.14 (1H, brs), 7.20-7.67 (9H, m), 8.07-5.17 (2H, m)

Example 4

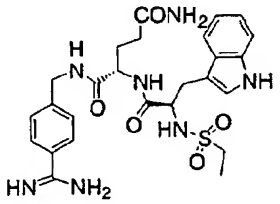
N-(Ethylsulfonyl)-1-(t-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide

[0155] To a solution of 1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (300 mg, 0.55 mmol) in DMF (10 ml), triethylamine (162 mg, 1.6 mmol) and ethanesulfonyl chloride (206 mg, 1.6 mmol) were added and stirred at room temperature under a nitrogen stream. After 12 hours, the solvent was distilled off under reduced pressure and the residue was applied to flash column chromatography (Merck Silicagel 60; mobile phase: dichloromethane:methanol = 10:1) to give N-(ethylsulfonyl) 1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (135 mg, 0.21 mmol; yield 38%).
H-NMR (CD_3OD) δ: 1.08 (3H, t, *J*=7 Hz), 1.70 (9H, s), 1.60-2.12 (4H, m), 2.75-3.34 (4H, m), 4.13-4.55 (4H, m), 7.24-7.78 (9H, m)

Example 5

N-(Ethylsulfonyl)-D-tryptophyl-N^1-(4-amidinobenzyl)-L-glutamide

[0156]



[0157] N-(Ethylsulfonyl)-1-(t-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (135 mg, 0.21 mmol) was dissolved in saturated hydrogen chloride/ethanol solution (10 ml) and allowed to stand at room temperature for 20 hours. After the solvent was removed under reduced pressure, the resulting N-(ethylsulfonyl)-D-tryptophyl-N^1-(4-ethoxyimino-carbonylbenzyl)-L-glutamide was dissolved in ethanol (8 ml) and further dissolved in ammonium acetate (500 mg, 6.4 mmol) and saturated ammonia/ethanol solution (1.3 ml), followed by heating at reflux. After 1 hour, the solvent was distilled off under reduced pressure and the residue was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane:methanol = 1:1) to give 4-amidino-[(S)-N-[(R)-N'-ethylsulfonyltryptophyl]glutaminyl]-aminomethylbenzene (94 mg, 0.17 mmol; yield 81%).
ESI+ 556 (M^++1)
H-NMR (DMSO-d6) δ: 0.85 (3H, t, *J*=7 Hz), 1.65-2.03 (2H, m), 2.48-3.54 (6H, m), 4.12-4.43 (4H, m), 6.70-7.75 (9H, m), 7.95 (1H, brs), 8.43 (2H, brs)

Example 6

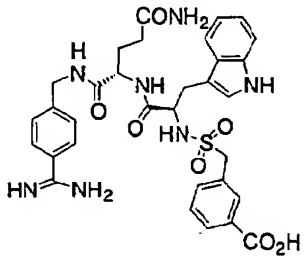
N-{[3-(Methoxycarbonyl)benzyl]sulfonyl}-1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzy)-L-glutamide

[0158] To a solution of 1-(t-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (350 mg, 0.64 mmol) in DMF (10 ml), triethylamine (194 mg, 1.9 mmol) and [3-(methoxycarbonyl)benzyl]sulfonyl chloride (477 mg, 1.9 mmol) were added and stirred at room temperature under a nitrogen stream. After 12 hours, the solvent was distilled off under reduced pressure and the residue was applied to flash column chromatography (Merck Silicagel 60; mobile phase: dichloromethane:methanol = 10:1) to give N-{[3-(methoxycarbonyl)benzyl]sulfonyl}-1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (407 mg, 0.21 mmol; yield 84%).
H-NMR (CD_3OD) δ: 1.70 (9H, s), 1.75-2.15 (4H, m), 2.65-3.42 (2H, m), 3.92 (3H, s), 3.88-4.54 (6H, m), 7.23-8.21 (13H, m)

Example7

N-[(3-(Carboxybenzyl)sulfonyl]-D-tryptophyl-N^1-(4-amidinobenzyl)-L-glutamide

[0159]



[0160] N-{[3-(Methoxycarbonyl)benzyl]sulfonyl}-1-(*t*-butoxycarbonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (407 mg, 0.21 mmol) was dissolved in saturated hydrogen chloride/ethanol solution (15 ml) and allowed to stand at room temperature for 20 hours. After the solvent was removed under reduced pressure, the resulting crude product was dissolved in ethanol (16 ml) and further dissolved in ammonium acetate (1 g, 12.8 mmol) and saturated ammonia/ethanol solution (2.4 ml), followed by heating at reflux. After 1 hour, the solvent was distilled off under reduced pressure and the residue was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane: methanol = 4:1, 1:1) to give a mixture of N-{[3-(methoxycarbonyl)benzyl]sulfonyl}-D-tryptophyl-N^1-(4-amidinobenzyl)-L-glutamide and N-{[3-(ethoxycarbonyl)-benzyl]sulfonyl}-D-tryptophyl-N^1-(4-amidinobenzyl)-L-glutamide. This mixture was dissolved in ethanol (2 ml), to which 2N aqueous sodium hydroxide (2 ml) was then added and stirred at room temperature. After 1 hour, the reaction mixture was adjusted to pH 6 with 1N aqueous hydrogen chloride and the precipitated product was collected by filtration. The resulting crude product was applied to preparative HPLC (YMC-pack ODS; gradient of 95% A/B to 45% A/B over 25 min, A = 0.1% TFA-H_2O, B = 0.1% TFA-CH_3CN) to give N-[(3-(carboxybenzyl)sulfonyl]-D-tryptophyl-N^1-(4-amidino-benzyl)-L-glutamide trifluoroacetate (68 mg, 0.088 mmol; yield 16%).
ESI+ 662 (M^++1)
H-NMR (DMSO-d6) δ: 1.64-2.02 (4H, m), 2.90-3.21 (2H, m), 3.89-4.41 (6H, m), 6.75-7.95 (13H, m)

Example 8

N-(Benzylsulfonyl)-D-isoleucine

[0161] To a solution of D-isoleucine (3 g, 22.9 mmol) in dioxane (184 ml), 1N aqueous sodium hydroxide (23 ml) and then benzylsulfonyl chloride (6 g, 34.4 mmol) were added and stirred at room temperature. After 3 hours, the reaction mixture was adjusted to pH 2 with 2N aqueous hydrogen chloride and then extracted with ethyl acetate. The ethyl acetate layer was dried over anhydrous magnesium sulfate. After magnesium sulfate was filtered off, the filtrate was concentrated under reduced pressure and the residue was applied to flash column chromatography (Merck Silicagel 60; mobile phase: dichloromethane:methanol = 10:1, 4:1) to give N-(benzyl-sulfonyl)-D-isoleucine (6.3 g, 22.2 mmol; yield 97%).

H-NMR ($CDCl_3$) δ: 0.78-1.02 (6H, m), 1.05-1.60 (2H, m), 1.68-1.92 (1H, m), 3.85 (1H, dd, *J*=4, 7 Hz), 4.22-4.38 (2H, m), 5.17 (1H, d, *J*=9 Hz), 5.97 (1H, brs), 7.26-7.48 (5H, m)

Example 9

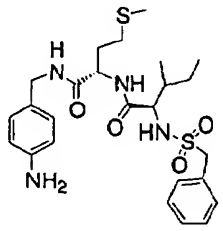
N-(Benzylsulfonyl)-D-isoleucyl-L-methionine methyl ester

[0162] To a solution of N-(benzylsulfonyl)-D-isoleucine (6.3 g, 22.2 mmol) and L-methionine methyl ester hydrochloride (6.7 g, 33.3 mmol) in dichloromethane (100 ml), HOBt (4.1 g, 26.6 mmol), EDC HCl (5.1 g, 1.2 mmol) and N-methylmorpholine (3.4 g, 33.3 mmol) were added and stirred at room temperature under a nitrogen stream After 12 hours, water was added to the reaction mixture, which was then extracted with ethyl acetate. The ethyl acetate layer was washed sequentially with 10% aqueous citric acid, saturated aqueous sodium bicarbonate and saturated brine, and then dried over anhydrous magnesium sulfate. After magnesium sulfate was filtered off, the filtrate was concentrated under reduced pressure and the residue was applied to flash column chromatography (Merck Silicagel 60; mobile phase: dichloromethane) to give N-(benzylsulfonyl)-D-isoleucyl-L-methionine methyl ester (6.4 g, 14.9 mmol; yield 67%).
H-NMR (CD_3OD) δ: 0.92-1.02 (6H, m), 1.18-1.36 (1H, m), 1.62-1.88 (2H, m), 2.00-2.28 (2H, m), 2.12 (3H, s), 2.51-2.77 (2H, m), 3.71 (3H, s), 3.83 (1H, d, *J*=8 Hz), 4.32 (2H, q, *J*= 13 Hz), 4.68 (1H, dd, *J*=5, 9 Hz), 7.32-7.51 (5H, m)

Example 10

N-(Benzylsulfonyl)-D-tryptophyl-N^1-(4-aminobenzyl)-L-methioninamide

[0163]



[0164] To a solution of N-(benzylsulfonyl)-D-isoleucyl-L-methionine methyl ester (6.4 g, 14.9 mmol) in ethanol (30 ml), 2N aqueous sodium hydroxide (30 ml) was added and stirred at room temperature. After 1 hour, the reaction mixture was adjusted to pH 2 with 2N aqueous hydrogen chloride and then extracted with ethyl acetate. The ethyl acetate layer was washed with saturated brine and then dried over anhydrous magnesium sulfate. Magnesium sulfate was filtered off and the filtrate was concentrated under reduced pressure to give N- (benzylsulfonyl) -D-isoleucyl-L-methionine (6.2 g, 14.9 mmol; yield 100%).
[0165] To a solution of N-(benzylsulfonyl)-D-isoleucyl-L-methionine (100 mg, 0.24 mmol) and 4-aminobenzylamine (59 mg, 0.48 mmol) in dichloromethane (5 ml), HOBt (44 mg, 0.29 mmol) and EDC HCl (56 mg, 0.29 mmol) were added and stirred at room temperature under a nitrogen stream. After 12 hours, the reaction mixture was concentrated under reduced pressure and water was added to the residue. The precipitated product was collected by filtration, washed with water and then dried. The resulting crude product was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane:methanol = 10:1) to give N-(benzyl-sulfonyl)-D-tryptophyl-N^1-(4-aminobenzyl) -L-methioninamide (108 mg, 0.21 mmol; yield 86%).
ESI+ 521 (M^++1)
H-NMR (CD_3OD) δ: 0.87-1.00 (6H, m), 1.09-1.28 (1H, m), 1.57-1.83 (2H, m), 1.86-2.26 (2H, m), 2.09 (3H, s), 2.43-2.69 (2H, m), 3.71 (3H, s), 4.13-4.32 (4H, m), 4.50-4.68 (2H, m), 6.64 (2H, d, *J*=8 Hz), 7.01 (2H, d, *J*=8 Hz), 7.32-7.49 (5H, m)

Example 11

N-(Propylsulfonyl) -D-isoleucyl-3-(methylamino-N^1-(4-cyanobenzyl)-L-alaninamide

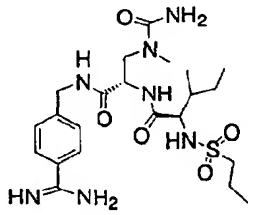
[0166] To N-(propylsulfonyl)-D-isoleucyl-3-[(*t*-butoxycarbonyl)(methyl)amino]-N^1-(4-cyanobenzyl)-L-alaninamide (1.6 g, 3 mmol), trifluoroacetic acid (10 ml) was added and stirred at room temperature under a nitrogen stream. After

1 hour, the reaction mixture was concentrated under reduced pressure and the residue was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane:methanol = 1:0, 4:1) to give N-(propylsulfonyl)-D-isoleucyl-3-(methylamino)-N^1-(4-cyanobenzyl)-L-alaninamide (1.3 g, 2.9 mmol, yield 96%).
ESI+ 452 (M^++1)
H-NMR ($CDCl_3$) δ: 0.79-1.23 (10H, m), 1.46-1.95 (4H, m), 2.41 (3H, s), 2.52-3.81 (4H, m), 4.33-4.52 (4H, m), 7.36 (2H, d, J=8 Hz), 7.59 (2H, d, J=8 Hz)

Example 12

N-(Propylsulfonyl)-D-isoleucyl-3-[(aminocarbonyl)(methyl)-amino]-N^1-(4-amidinobenzyl)-L-alaninamide

[0167]



[0168] To a solution of N-(propylsulfonyl)-D-isoleucyl-3-(methylamino)-N^1-(4-cyanobenzyl)-L-alaninamide (500 mg, 1.0 mmol) in water (1.3 ml)/tetrahydrofuran (3 ml), potassium cyanate (243 mg, 3 mmol) was added under stirring at 50°C and then further stirred under the same conditions. After stirring for 3 hours, water was added to the reaction mixture, which was then extracted with ethyl acetate. The ethyl acetate layer was dried over anhydrous magnesium sulfate. Magnesium sulfate was filtered off and the filtrate was concentrated under reduced pressure to give N-(propylsulfonyl)-D-isoleucyl-3-[(aminocarbonyl)(methyl)amino]-N^1-(4-cyanobenzyl)-L-alaninamide (430 mg, 0.87 mmol; yield 87%).
[0169] The resulting product was dissolved in saturated hydrogen chloride/ethanol solution (10 ml) and allowed to stand at room temperature for 20 hours. After the solvent was removed under reduced pressure, the resulting crude product was dissolved in saturated ammonia/ethanol solution (10 ml) and allowed to stand at room temperature for 20 hours. The solvent was distilled off under reduced pressure and the residue was applied to preparative HPLC (YMC-pack ODS: gradient of 95% A/B to 25% A/B over 10 min, A = 0.1% TFA-H_2O, B = 0.1% TFA-CH_3CN) to give N-(propylsulfonyl)-D-isoleucyl-3-[(aminocarbonyl)-(methyl)amino]-N^1-(4-amidinobenzyl)-L-alaninamide trifluoroacetate (27 mg, 0.004 mmol; yield 5%).
ESI+ 512 (M^++1)
H-NMR (CD3OD) δ: 0.87-1.10 (9H, m), 1.12-1.88 (5H, m), 2.92 (3H, s), 2.87-3.12 (2H, m), 3.52 (1H, dd, *J*=4, 15 Hz), 3.65 (1H, d, *J*=8 Hz), 3.82 (1H, dd, *J*=9, 14 Hz), 4.43-4.67 (3H, m), 7.54 (2H, d, *J*=8 Hz), 7.76 (2H, d, *J*=8 Hz)

Example 13

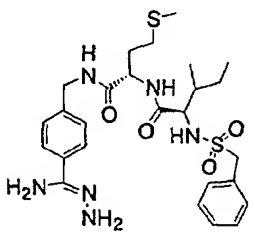
N-(Benzylsulfonyl)-D-isoleucyl-N^1-{4-[imino(methylthio)-methyl]benzyl}-L-methioninamide

[0170] N-(Benzylsulfonyl)-D-isoleucyl-N^1-(4-cyanobenzyl)-L-methioninamide (100 mg, 0.19 mmol) was dissolved in pyridine (5 ml) and triethylamine (0.5 ml), bubbled with a hydrogen sulfide gas for 5 minutes, and then stirred for 24 hours. After addition of ethyl acetate to the reaction mixture, the organic layer was washed sequentially with 0.5 N hydrochloric acid, saturated aqueous sodium bicarbonate and saturated brine, and then dried over sodium sulfate. The solvent was distilled off under reduced pressure and the residue was dissolved in acetonitrile, followed by addition of methyl iodide (0.14 ml, 0.94 mmol) and heating at reflux for 2 hours under a nitrogen atmosphere. The solvent was distilled off under reduced pressure and the residue was purified on a silica gel column (dichloromethane:methanol = 10:1) to give N-(benzyl-sulfonyl)-D-isoleucyl-N^1-{4-[imino(methylthio)methyl]benzyl}-L-methioninamide (109 mg, 0.19 mmol; yield 100%).
ESI+ 579 (M^++1)
H-NMR (CD_3OD) δ: 0.85-0.90 (6H, m), 2.03 (3H, s), 2.40 (3H, s), 3.69 (1H, t, J=6 Hz), 4.50-4.60 (1H, m), 7.21-7.39 (8H, m), 7.60-7.64 (1H, m)

Example 14

N-(Benzylsulfonyl)-D-isoleucyl-N^1-{4-[hydrazino(imino)-methyl]benzyl}-L-methioninamide

[0171]

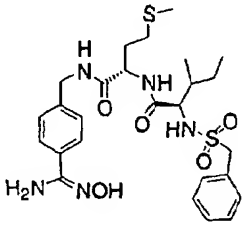


[0172] N-(Benzylsulfonyl)-D-isoleucyl-N^1-{4-[imino-(methylthio)methyl]benzyl}-L-methioninamide (49 mg, 0.084 mmol) was dissolved in dichloromethane (2 ml) and methanol (2 ml), to which hydrazine (0.020 ml, 0.624 mmol) was then added and stirred for 18 hours. The solvent was distilled off under reduced pressure and the residue was purified by preparative HPLC to give N-(benzylsulfonyl)-D-isoleucyl-N^1-{4-[hydrazino(imino)methyl]benzyl}-L-methioninamide (29 mg, 0.051 mmol; yield 61%).
ESI+ 563 (M^++1)
H-NMR (CD_3OD) δ: 0.85-0.90 (6H, m), 1.58-1.78 (2H, m), 2.42-2.58 (2H, m), 3.63 (1H, d, *J*=7 Hz), 4.21 (2H, s), 4.53 (1H, brs), 7.25-7.57 (9H, m)

Example 15

N-(Benzylsulfonyl)-D-isoleucyl-N^1-[4-(E)-amino-(hydroxyimino)methyl]benzyl]-L-methioninamide

[0173]

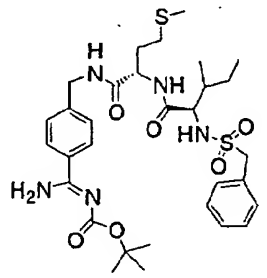


[0174] N-(Benzylsulfonyl)-D-isoleucyl-N^1-(4-cyanobenzyl)-L-methioninamide (100 mg, 0.19 mmol) was dissolved in ethanol (6 ml) and pyridine (0.6 ml), to which hydroxyamine hydrochloride (120 mg) was then added and stirred for 16 hours. After the solvent was distilled off under reduced pressure, the residue was dissolved in ethanol, filtered and then purified by preparative HPLC to give N-(benzylsulfonyl)-D-isoleucyl-N^1-[4-(E)-amino(hydroxyimino)methyl]benzyl] -L-methioninamide (1.6 mg, 0.00003 mmol; yield 1.5%).
ESI+ 564 (M^++1)
H-NMR (CD_3OD) δ: 0.85-0.90 (6H, m), 1.50-1.70 (2H, m), 2.05 (3H, s), 2.43-2.60 (2H, m), 3.60 (1H, d, *J*=8 Hz), 4.20 (1H, s), 7.25-7.45 (9H, m)

Example 16

N-(Benzylsulfonyl)-D-isoleucyl-N^1-[4-((E)-amino{[(*t*-butyloxy)carbonyl]imino}methyl)benzyl]-L-methioninamide

[0175]



[0176] N-(Benzylsulfonyl)-D-isoleucyl-N^1-{4-[amino(imino)-methyl]benzyl}-L-methioninamide (20 mg, 0.032 mmol) was dissolved in dimethylformamide (0.5 ml), to which triethylamine (0.018 ml, 0.13 mmol) and di-t-butyl carbonate (14 mg, 0.065 mmol) were then added and stirred for 16 hours. After addition of ethyl acetate to the reaction mixture, the organic layer was washed with water and dried over sodium sulfate. The solvent was distilled off under reduced pressure and the residue was purified by preparative TLC (dichloromethane:methanol = 10:1) to give N-(benzylsulfonyl) -D-isoleucyl-N^1-[4-((E)-amino-[[(t-butyloxy)carbonyl]imino]methyl)benzyl]-L-methioninaniide (16 mg, 0.024 mmol; yield 76%).
ESI+ 648 (M^++1)
H-NMR (CD_3OD) δ: 0.85-0.90 (6H, m), 1.50 (9H, s), 2.03 (3H, s), 3.68 (1H, d, *J*=8 Hz), 4.20 (2H, s), 7.20-7.38 (7H, m), 7.64-7.70 (2H, m)

Example 17

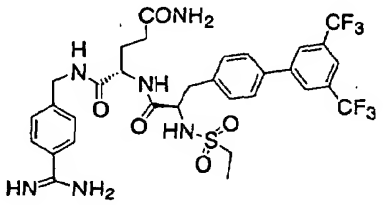
N-(Ethylsulfonyl)-3,5-bis(trifluoromethyl)-D-phenylalanyl-N^1-4-cyanobenzyl)-L-glutamide

[0177] 4-Bromo-N-(ethylsulfonyl)-D-phenylalanyl-N^1-(4-cyanobenzyl)-L-glutamide (30 mg, 0.052 mmol) was dissolved in tetrahydrofuran (4 ml) and water (0.4 ml). Subsequently, 3,5-bistrifluoromethylphenylboronic acid (40.2 mg, 0.156 mmol), sodium carbonate (50 mg) and tetrakis(triphenylphosphine)-palladium (30 mg, 0.026 mmol) were added to the solution, followed by heating at reflux for 2 hours under a nitrogen atmosphere. After addition of ethyl acetate to the reaction mixture, the organic layer was washed with water and dried over sodium sulfate. The solvent was distilled off under reduced pressure and the residue was purified by preparative TLC (dichloromethane:methanol = 10:1) and then preparative HPLC to give N-(ethylsulfonyl)-3,5-bis(trifluoromethyl)-D-phenylalanyl-N^1-(4-cyanobenzyl)-L-glutamide (24 mg, 0.034 mmol; yield 65%).
ESI+ 712 (M^++1)
H-NMR (CD_3O) δ: 1.10 (3H, t, *J*=7 Hz), 1.75-1.87 (2H, m), 1.88-2.07 (2H, m), 2.82-3.10 (4H, m), 4.10-4.30 (2H, m), 4.40-4.50 (2H, m), 7.10-7.62 (9H, m), 8.10 [1H, s)

Example 18

N-(Ethylsulfonyl)-3,5-bis(trifluoromethyl)-D-phenylalanyl-N^1-{4-amidinobenzyl}-L-glutamide

[0178]



[0179] Starting with N-(ethylsulfonyl)-3,5-bis(trifluoromethyl)-D-phenylalanyl-N'-(4-cyanobenzyl)-L-glutamide, the same procedure as shown in Example 5 was repeated to give the compound of interest.
ESI+ 729 (M^++1)
H-NMR (CD_3OD) δ: 1.05 (3H, t, *J*=7 Hz), 1.75-1.85 (2H, m), 1.97-2.05 (2H, m), 2.82-3.10 (4H, m), 4.15-4.22 (2H, m), 4.45 (1H, s), 7.40-7.51 (4H, m), 7.62-7.70 (3H, m), 7.90 (1H, s), 8.13 (2H, s)

Example 19

N-(*t*-Butoxycarbonyl)-5-{[3-(methoxycarbonyl)-5-benzyl]oxy}-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide

[0180] To a solution of N-(*t*-butoxycarbonyl)5-hydroxy-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (327 mg, 0.58 mmol) in acetone (4 ml), 3-(methoxycarbonyl)benzylbromide (267 mg, 1.2 mmol) and cesium carbonate (378 mg, 1.2 mmol) were added and stirred at reflux under a nitrogen stream. After 4 hours, the reaction mixture was filtered and the filtrate was concentrated under reduced pressure. The residue was applied to flash column chromatography (Merck Silicagel 60; mobile phase: dichloromethane:methanol = 10:1) to give N-(*t*-butoxycarbonyl)-5-{[3-(methoxycarbonyl) benzyl]oxy}-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (347 mg, 0.5 mmol; yield 84%).
ESI+ 711 (M^++1)
H-NMR (CD_3OD) δ: 1.30 (9H, s), 1.50-2.08 (4H, m), 3.02-3.22 (2H, m), 3.93 (3H, s), 4.02-4.27 (2H, m), 4.39-4.55 (1H, m), 5.20 (2H, s), 6.88 (1H, dd, *J*=2, 9 Hz), 7.12 (1H, s), 7.19 (1H, d, *J*=2 Hz), 7.26 (1H, d, *J*=9 Hz), 7.42 (2H, d, *J*=8 Hz), 7.51 (1H, t, *J*=7 Hz), 7.66 (2H, d, *J*=8 Hz), 7.75 (1H, d, *J*=6 Hz), 7.97 (1H, d, *J*=6 Hz), 8.17 (1H, s)

Example 20

5-{[3-(Methoxycarbonyl)benzyl]oxy}-N-(ethylsulfonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide

[0181] To a solution of N-(*t*-butoxycarbonyl)-5-{[3-(methoxycarbonyl)benzyl]oxy}-D-tryptophyl-N^1-(4-cyanobenzyl) -L-glutamide (347 mg, 0.5 mmol) in dichloromethane (10 ml), trifluoroacetic acid (10 ml) was added and stirred at room temperature under a nitrogen stream. After 1 hour, the solvent was distilled off under reduced pressure. The residue was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane:methanol = 1:1) to give 5-{[3-(methoxycarbonyl)benzyl]oxy}-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (277 mg, 0.45 mmol; yield 93%).

[0182] To a solution of 5-{[3-(methoxycarbonyl)benzyl]oxy}-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (0.45 mmol) in DMF (10 ml), triethylamine (137 mg, 1.4 mmol) and ethanesulfonyl chloride (174 mg, 1.4 mmol) were added and stirred at room temperature under a nitrogen stream. After 2 hours, the solvent was distilled off under reduced pressure and the residue was applied to flash column chromatography (Merck Silicagel 60; mobile phase: dichloromethane:methanol=8:1) to give 5-{[3-(methoxycarbonyl)benzyl]oxy}-N-(ethylsulfonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (158 mg, 0.22 mmol; yield 50%).
ESI+ 703 (M^++1)
H-NMR (CD_3OD) δ: 0.94 (3H, t, *J*=7 Hz), 1.60-2.08 (4H, m), 2.58-3.30 (4H, m), 3.91 (3H, s), 4.02-4.27 (2H, m), 4.35-4.48 (2H, m), 5.20 (2H, s), 6.89 (1H, dd, *J*=2, 9 Hz), 7.12 (1H, s), 7.19 (1H, d, *J*=2 Hz), 7.27 (1H, d, *J*=9 Hz), 7.42-7.53 (3H, m), 7.65 (2H, d, *J*=8 Hz), 7.73 (1H, d, *J*=6 Hz), 7.98 (1H, d, *J*=6 Hz), 8.16 (1H, s)

Example 21

5-{[3-(Methoxycarbonyl)benzyl]oxy}-N (ethylsulfonyl)-D-tryptophyl-N^1-{4-[amino(imino)methyl]benzyl}-L-glutamide

[0183] A solution of 5-{[3-(methoxycarbonyl)benzyl]oxy}-N-(ethylsulfonyl)-D-tryptophyl-N^1-(4-cyanobenzyl)-L-glutamide (158 mg, 0.22 mmol) in pyridine (10 ml) and triethylamine (2 ml) was bubbled with a hydrogen sulfide gas. After bubbling for 30 minutes, the solution was allowed to stand. After 12 hours, water/ethyl acetate was added to the reaction mixture and the aqueous layer was adjusted to pH 4 with 2N aqueous hydrogen chloride, followed by extraction. The organic layer was washed with saturated brine and then dried over anhydrous magnesium sulfate. Magnesium sulfate was filtered off and the filtrate was concentrated under reduced pressure.

[0184] The residue was dissolved in acetone (10 ml), to which methyl iodide (312 mg, 2.2 mmol) was then added and stirred at 50°C under a nitrogen stream. After 1 hour, the reaction mixture was concentrated under reduced pressure.

[0185] The residue was dissolved again in methanol (10 ml), followed by addition of ammonium acetate (170 mg, 2.2 mmol) and heating at reflux under a nitrogen stream. After 4 hours, the solvent was distilled off under reduced pressure and the residue was applied to column chromatography (Fuji Silysia NH-DM-1020; mobile phase: dichloromethane:methanol = 4:1, 2:1) to give 5-{[3-(methoxycarbonyl)benzyl]oxy}-N-(ethylsulfonyl)-D-tryptophyl-N^1-{4-[amino(imino)methyl]benzyl}-L-glutamide (124 mg, 0.17 mmol; yield 78%).

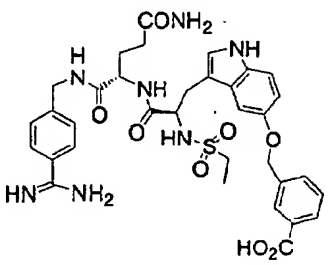
ESI+ 720 (M^++1)

H-NMR (CD_3OD) δ: 0.94 (3H, t, *J*=7 Hz), 1.64-2.10 (4H, m), 2.55-3.30 (4H, m), 3.89 (3H, s), 4.08-4.42 (4H, m), 5.18 (2H, s), 6.87 (1H, dd, *J*=2, 9 Hz), 7.15 (1H, s), 7.20-7.76 (8H, m), 7.95 (1H, d, *J*=6 Hz), 8.14 (1H, s)

Example 22

5-[(3-Carboxybenzyl)oxy]-N-(ethylsulfonyl)-D-tryptophyl-N^1-{4-[amino(imino)methyl]benzyl}-L-glutamide

[0186]



[0187] To a solution of 5-{[3-(methoxycarbonyl)benzyl]oxy}-N-(ethylsulfonyl)-D-tryptophyl-N^1-{4-[amino(imino)methyl]-benzyl}-L-glutamide (124 mg, 0.17 mmol) in ethanol (3 ml), 1N aqueous sodium hydroxide (3 ml) was added and stirred at room temperature. After 2 hours, the reaction mixture was adjusted to pH 6 with 1N aqueous hydrogen chloride and then concentrated under reduced pressure. The residue was applied to preparative HPLC (YMC-pack ODS: gradient of 95% A/B to 25% A/B over 10 min, A = 0.1% TFA-H_2O, B = 0.1% TFA-CH_3CN) to give 5-[(3-carboxybenzyl)oxy]-N-(ethylsulfonyl)-D-tryptophyl-N^1-{4-[amino(imino)methyl]benzyl}-L-glutamide (85 mg, 0.1 mmol; yield 61%).

ESI+ 706 (M^++1)

H-NMR (CD_3OD) δ: 0.97 (3H, t, *J*=7 Hz), 1.59-2.07 (4H, m), 2.55-3.28 (4H, m), 3.89 (3H, s), 4.10-4.54 (4H, m), 5.19 (2H, s), 6.90 (1H, dd, *J*=2, 9 Hz), 7.16 (1H, s), 7.23 (1H, d, *J*=2 Hz), 7.27 (1H, d, *J*=9 Hz), 7.50-8.00 (7H, m), 8.16 (1H, s)

Examples 23 to 182

[0188] The compounds of Examples 23 to 182 were prepared according to Examples 1 to 22 and the reaction schemes mentioned above. Tables 1 to 34 summarize the chemical structures and instrumental analysis data of these compounds. In the tables, Reagent 2, Reagent 5, Intermediate 9 and others are the same as the corresponding reagents and intermediates shown in the above reaction schemes.

Table 1

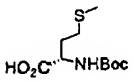
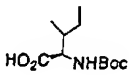
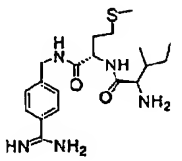
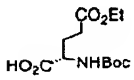
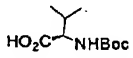
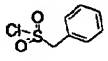
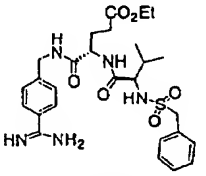
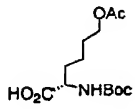
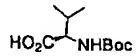
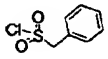
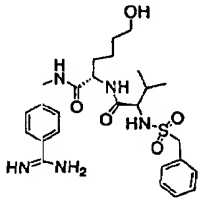
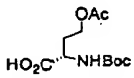
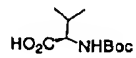
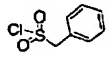
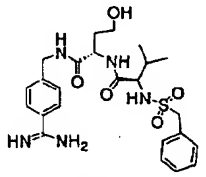
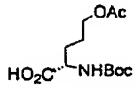
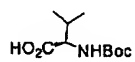
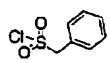
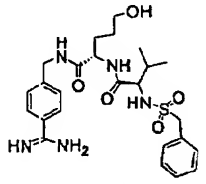
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
23				 ESI+ 394 (M^++1)
24				 FAB+ 560 (M^++1)
25				 FAB+ 532 (M^++1)
26				 ESI+ 504 (M^++1)
27				 FAB+ 518 (M^++1)

Table 2

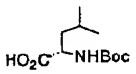
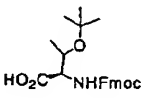
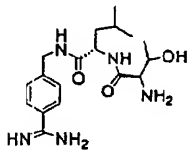
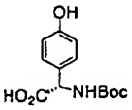
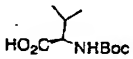
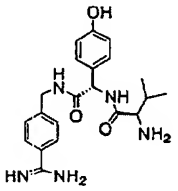
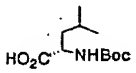
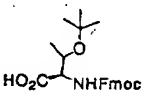
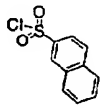
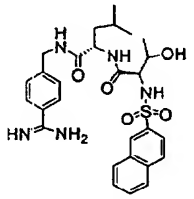
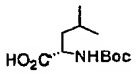
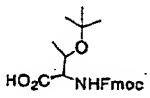
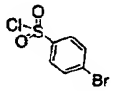
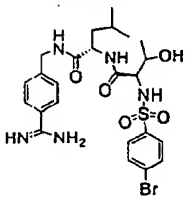
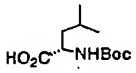
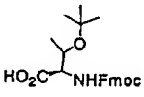
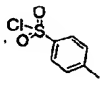
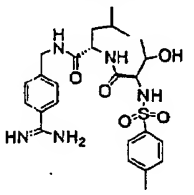
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
28				 FAB+ 364 (M^++1)
29				 ESI+ 398 (M^+)
30				 ESI+ 554 (M^++1)
31				 ESI+ 583 (M^++1)
32				 ESI+ 518 (M^++1)

Table 3

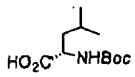
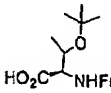
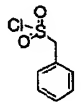
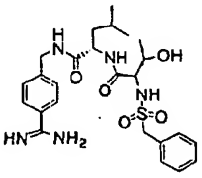
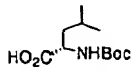
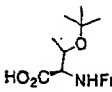
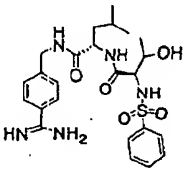
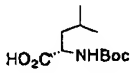
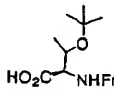
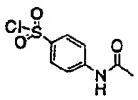
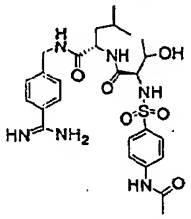
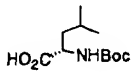
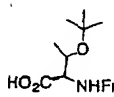
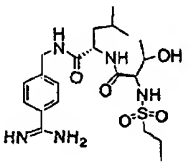
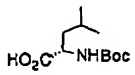
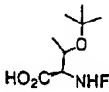
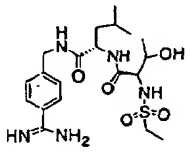
Example	Reagent 2	Reagent 5	Reagent 6	Structure MS
33				 ESI+ 518 (M^++1)
34				 ESI+ 504 (M^++1)
35				 ESI+ 561 (M^++1)
36				 ESI+ 470 (M^++1)
37				 ESI+ 456 (M^++1)

Table 4

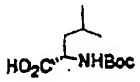
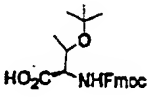
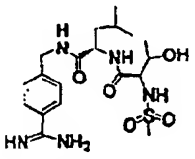
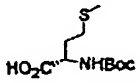
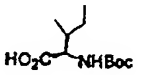
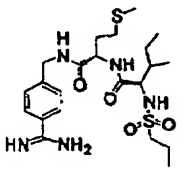
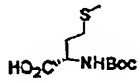
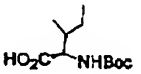
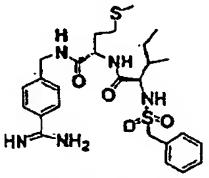
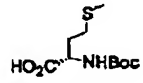
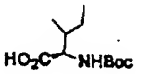
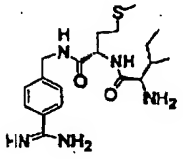
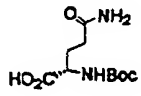
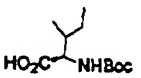
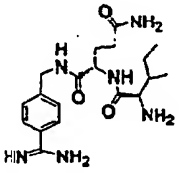
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
38				 ESI+ 442 (M^++1)
39				 FAB+ 500 (M^++1)
40				 FAB+ 548 (M^++1)
41				 FAB+ 394 (M^++1)
42				 FAB+ 391 (M^++1)

Table 5

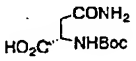
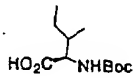
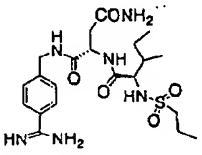
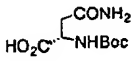
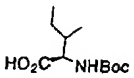
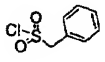
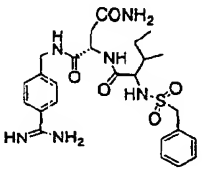
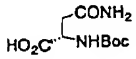
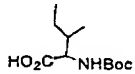
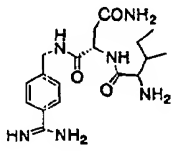
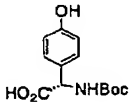
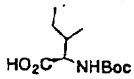
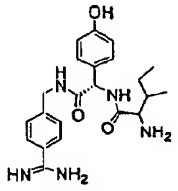
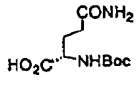
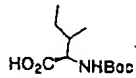
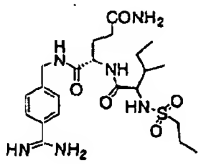
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
43				 FAB+ 483 (M^++1)
44				 FAB+ 531 (M^++1)
45				 ESI+ 377 (M^++1)
46				 FAB+ 412 (M^++1)
47				 FAB+ 497 (M^++1)

Table 6

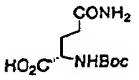
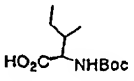
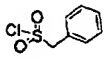
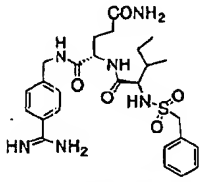
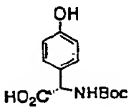
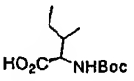
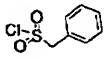
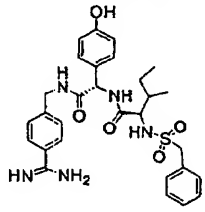
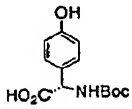
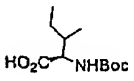
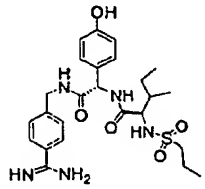
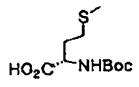
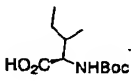
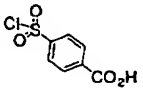
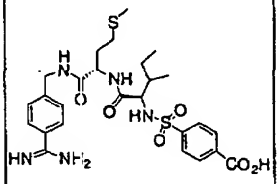
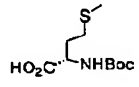
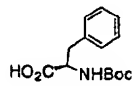
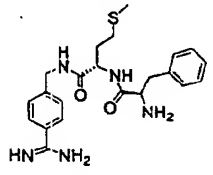
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
48				 FAB+ 526 (M^++1)
49				 FAB+ 566 (M^++1)
50				 ESI+ 518 (M^++1)
51				 ESI+ 578 (M^++1)
52				 FAB+ 428 (M^++1)

Table 7

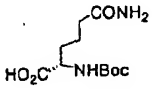
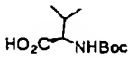
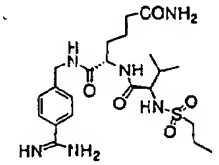
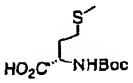
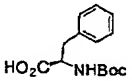
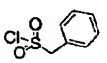
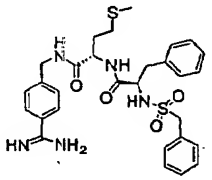
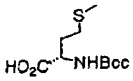
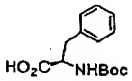
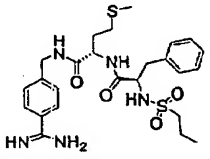
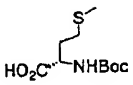
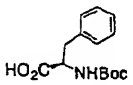
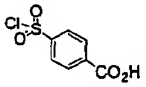
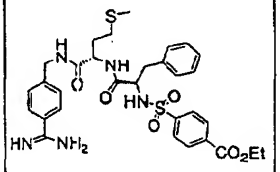
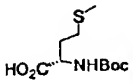
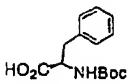
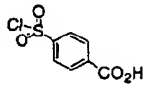
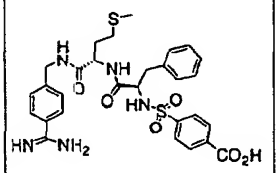
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
53				 FAB+ 497 (M^++1)
54				 FAB+ 582 (M^++1)
55				 FAB+ 534 (M^++1)
56				 ESI+ 640 (M^++1)
57				 ESI+ 612 (M^++1)

Table 8

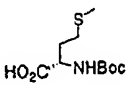
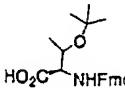
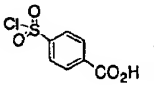
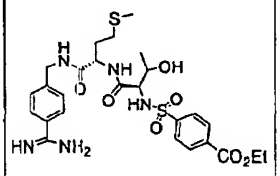
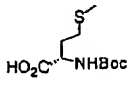
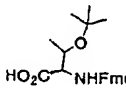
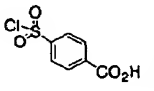
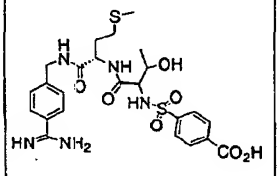
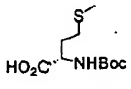
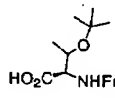
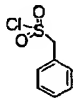
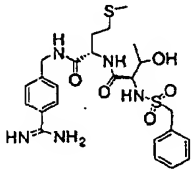
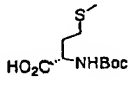
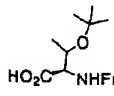
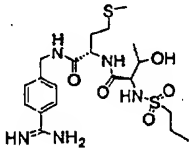
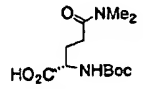
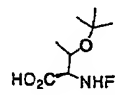
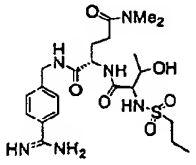
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
58				 ESI+ 594 (M^++1)
59				 ESI+ 556 (M^++1)
60				 ESI+ 536 (M^++1)
61				 ESI+ 488 (M^++1)
62				 FAB+ 513 (M^++1)

Table 9

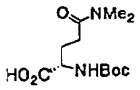
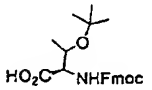
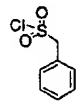
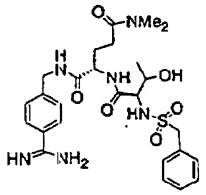
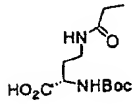
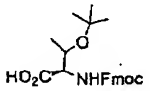
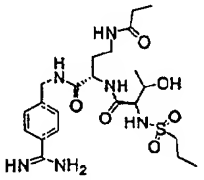
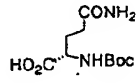
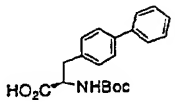
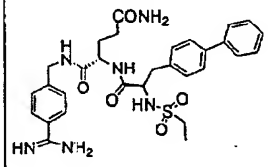
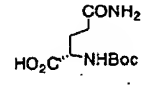
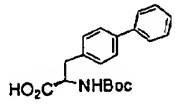
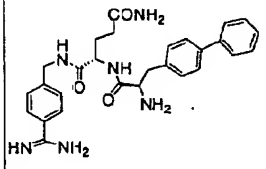
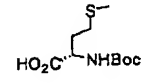
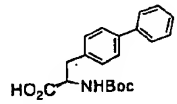
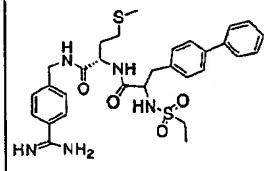
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
63				 FAB+ 561 (M^++1)
64				 ESI+ 512 (M^++1)
65				 ESI+ 593 (M^++1)
66				 ESI+ 501 (M^++1)
67				 ESI+ 596 (M^++1)

Table 10

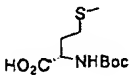
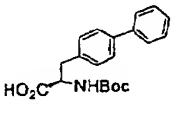
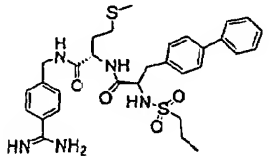
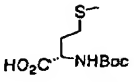
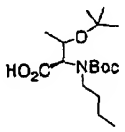
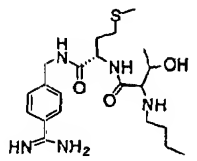
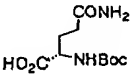
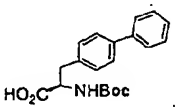
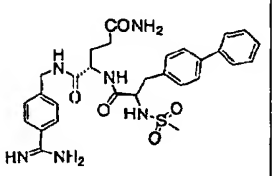
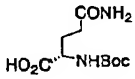
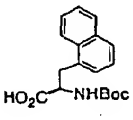
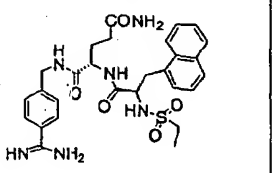
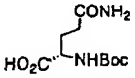
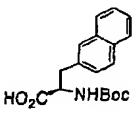
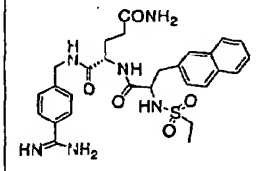
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
68				 ESI+ 610 (M^++1)
69				 ESI+ 438 (M^++1)
70				 ESI+ 579 (M^++1)
71				 ESI+ 567 (M^++1)
72				 ESI+ 567 (M^++1)

Table 11

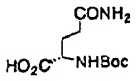
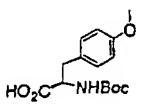
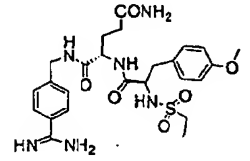
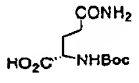
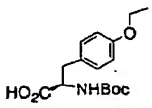
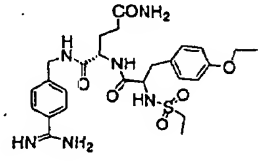
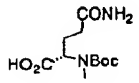
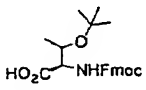
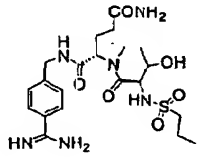
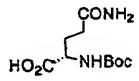
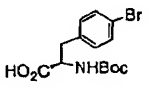
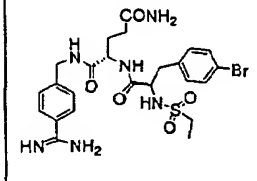
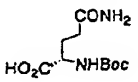
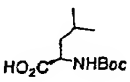
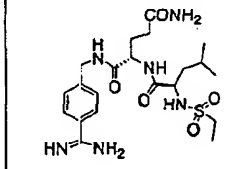
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
73				 ESI+ 547 (M^++1)
74				 ESI+ 561 (M^++1)
75				 ESI+ 599 (M^++1)
76				 ESI+ 595 (M^++1)
77				 ESI+ 483 (M^++1)

Table 12

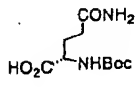
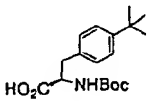
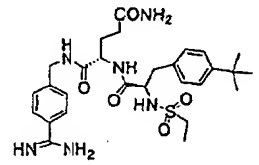
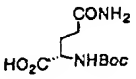
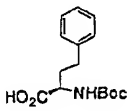
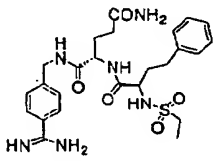
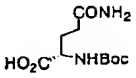
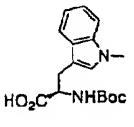
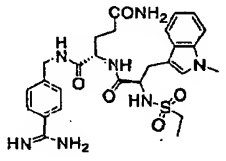
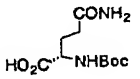
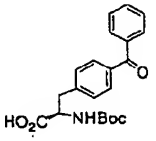
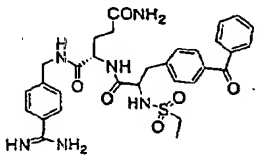
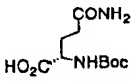
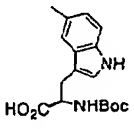
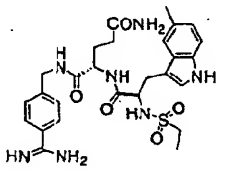
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
78				 ESI+ 573 (M^++1)
79				 ESI+ 531 (M^++1)
80				 ESI+ 570 (M^++1)
81				 ESI+ 621 (M^++1)
82				 ESI+ 570 (M^++1)

Table 13

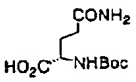
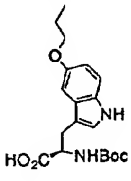
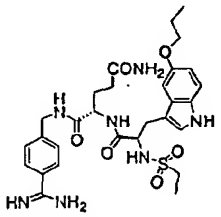
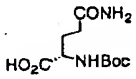
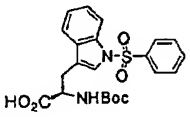
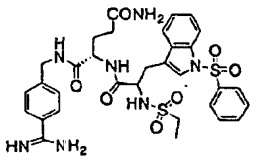
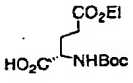
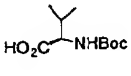
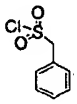
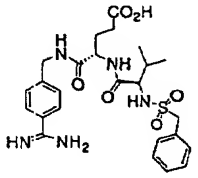
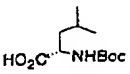
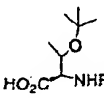
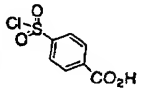
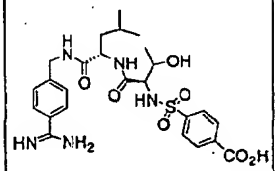
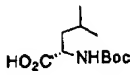
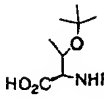
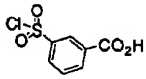
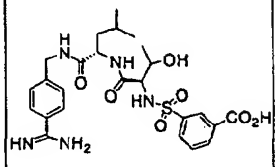
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
83				 ESI+ 614 (M^++1)
84				 ESI+ 696 (M^++1)
85				 FAB+ 532 (M^++1)
86				 FAB+ 548 (M^++1)
87				 FAB+ 548 (M^++1)

Table 14

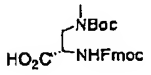
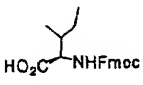
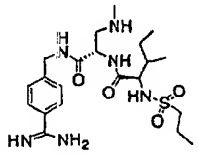
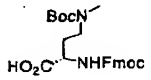
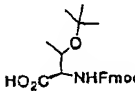
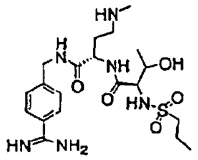
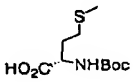
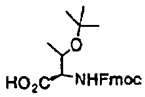
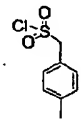
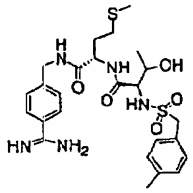
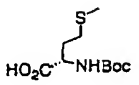
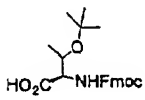
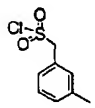
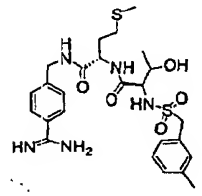
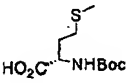
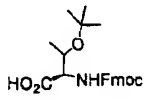
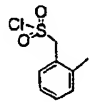
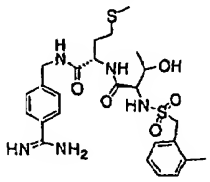
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
88				 ESI+ 469 (M^++1)
89				 ESI+ 471 (M^++1)
90				 ESI+ 550 (M^++1)
91				 ESI+ 550 (M^++1)
92				 ESI+ 550 (M^++1)

Table 15

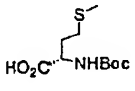
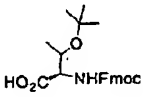
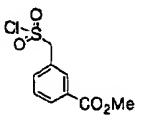
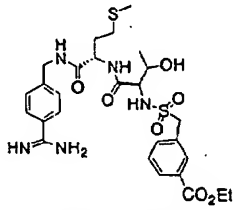
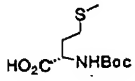
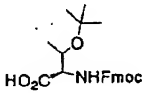
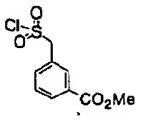
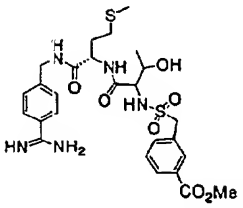
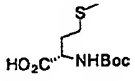
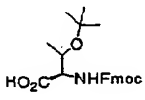
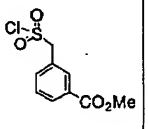
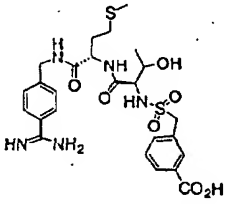
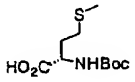
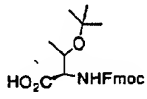
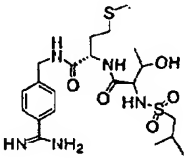
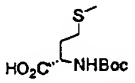
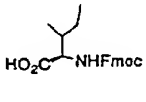
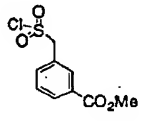
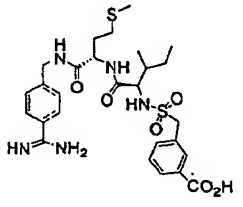
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
93				 ESI+ 608 (M^++1)
94				 ESI+ 594 (M^++1)
95				 ESI+ 580 (M^++1)
96				 ESI+ 502 (M^++1)
97				 ESI+ 592 (M^++1)

Table 16

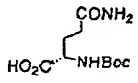
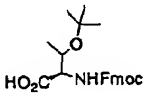
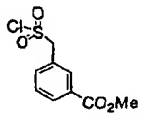
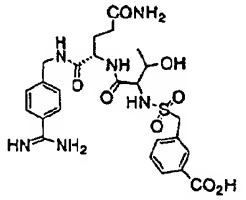
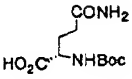
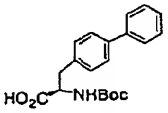
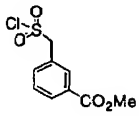
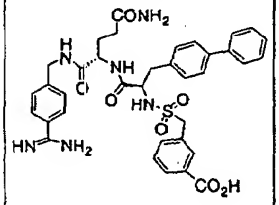
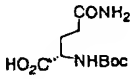
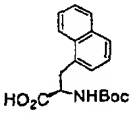
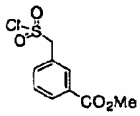
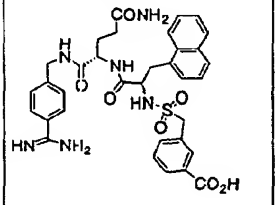
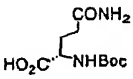
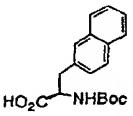
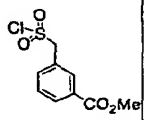
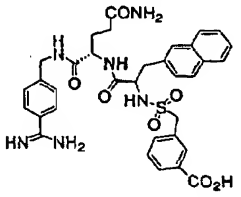
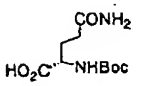
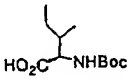
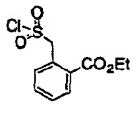
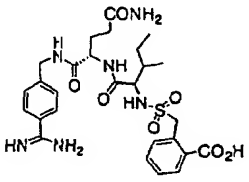
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
98				 ESI+ 577 (M^++1)
99				 ESI+ 699 (M^++1)
100				 ESI+ 673 (M^++1)
101				 ESI+ 673 (M^++1)
102				 ESI+ 589 (M^++1)

Table 17

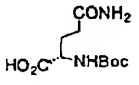
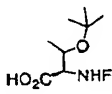
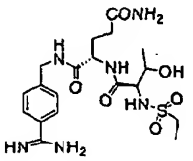
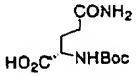
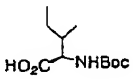
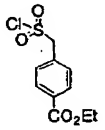
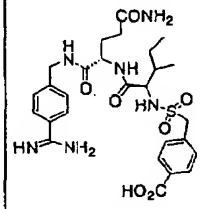
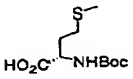
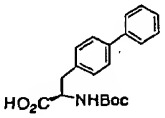
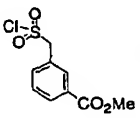
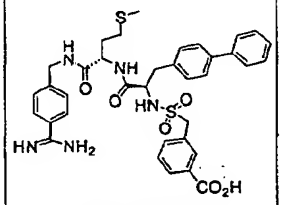
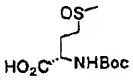
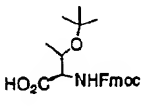
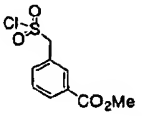
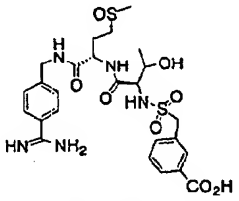
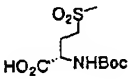
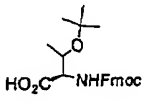
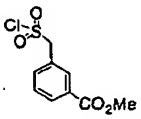
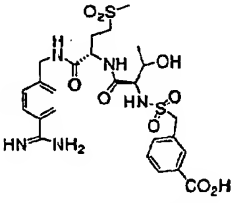
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
103				 ESI+ 471 (M^++1)
104				 ESI+ 589 (M^++1)
105				 ESI+ 702 (M^++1)
106				 ESI+ 596 (M^++1)
107				 ESI+ 612 (M^++1)

Table 18

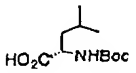
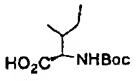
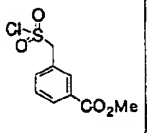
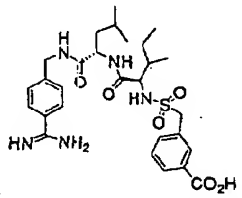
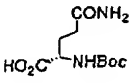
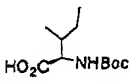
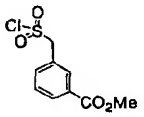
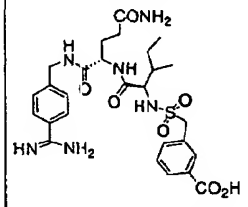
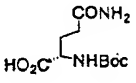
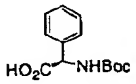
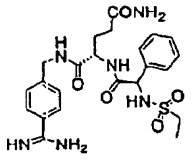
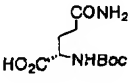
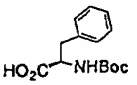
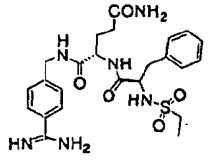
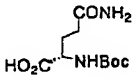
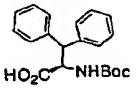
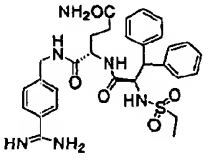
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
108				 ESI+ 574 (M^++1)
109				 ESI+ 589 (M^++1)
110				 ESI+ 503 (M^++1)
111				 ESI+ 517 (M^++1)
112				 ESI+ 593 (M^++1)

Table 19

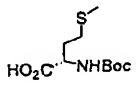
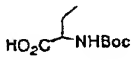
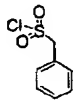
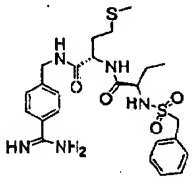
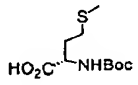
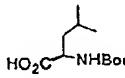
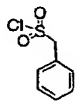
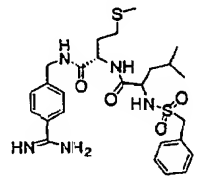
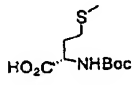
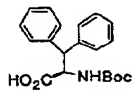
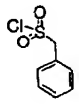
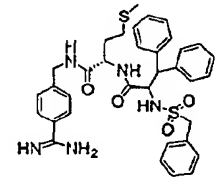
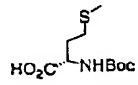
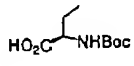
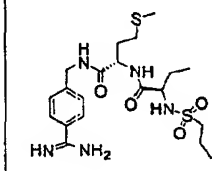
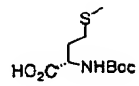
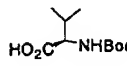
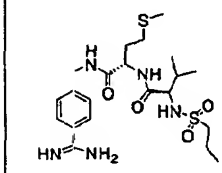
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
113				 ESI+ 520 (M^++1)
114				 ESI+ 548 (M^++1)
115				 ESI+ 658 (M^++1)
116				 ESI+ 472 (M^++1)
117				 ESI+ 486 (M^++1)

Table 20

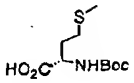
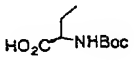
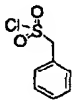
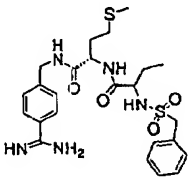
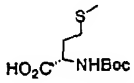
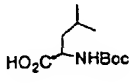
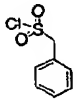
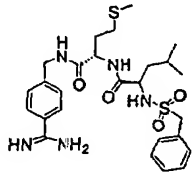
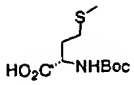
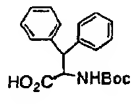
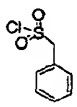
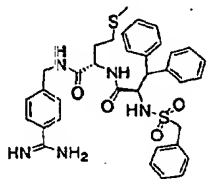
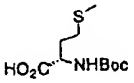
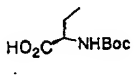
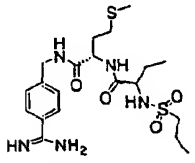
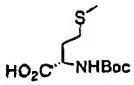
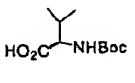
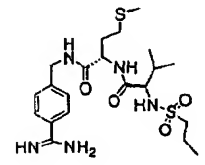
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
113				 ESI+ 520 (M^++1)
114				 ESI+ 548 (M^++1)
115				 ESI+ 658 (M^++1)
116				 ESI+ 472 (M^++1)
117				 ESI+ 486 (M^++1)

Table 21

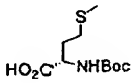
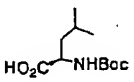
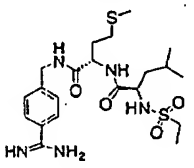
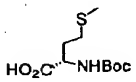
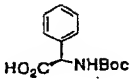
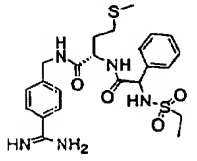
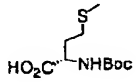
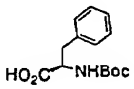
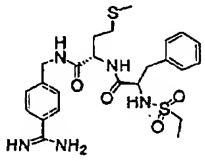
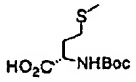
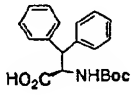
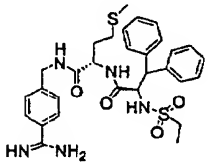
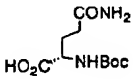
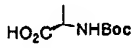
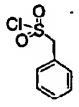
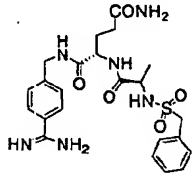
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
123				 ESI+ 486 (M^++1)
124				 ESI+ 506 (M^++1)
125				 ESI+ 520 (M^++1)
126				 ESI+ 596 (M^++1)
127				 ESI+ 503 (M^++1)

Table 22

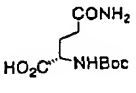
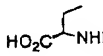
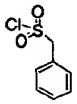
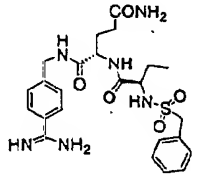
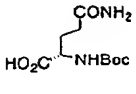
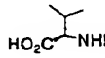
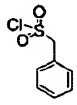
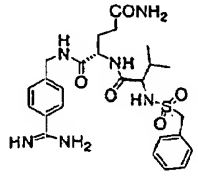
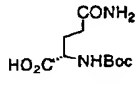
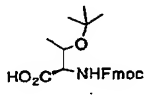
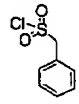
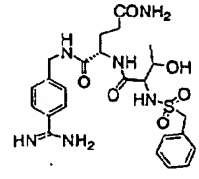
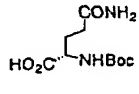
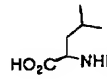
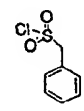
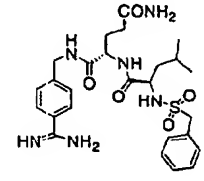
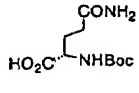
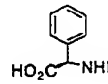
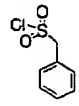
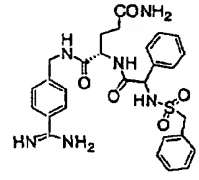
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
128				 ESI+ 517 (M^++1)
129				 ESI+ 531 (M^++1)
130				 ESI+ 593 (M^++1)
131				 ESI+ 545 (M^++1)
132				 ESI+ 565 (M^++1)

Table 23

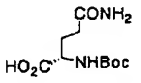
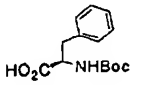
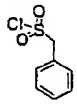
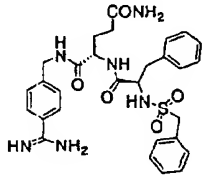
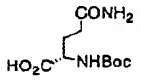
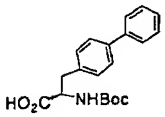
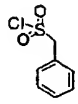
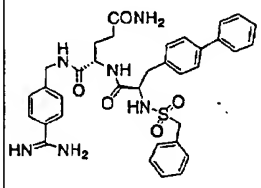
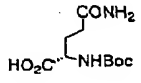
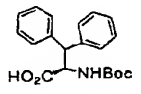
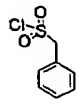
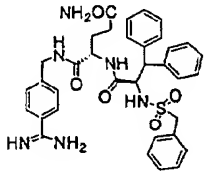
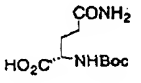
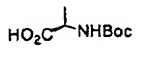
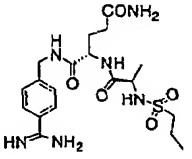
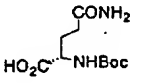
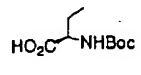
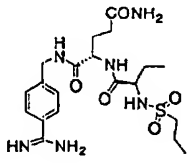
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
133				 ESI+ 579 (M^++1)
134				 ESI+ 655 (M^++1)
135				 ESI+ 655 (M^++1)
136				 ESI+ 455 (M^++1)
137				 ESI+ 469 (M^++1)

Table 24

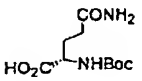
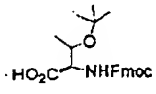
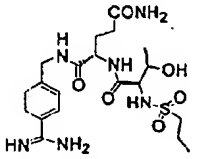
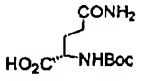
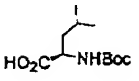
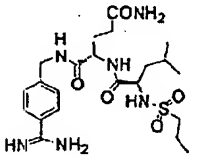
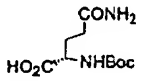
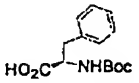
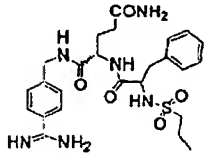
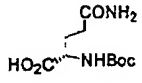
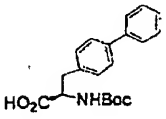
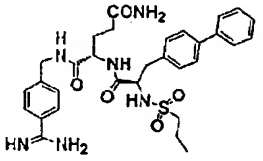
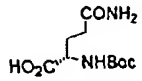
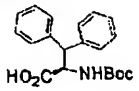
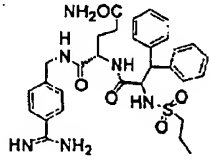
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
138				 ESI+ 485 (M^++1)
139				 ESI+ 497 (M^++1)
140				 ESI+ 531 (M^++1)
141				 ESI+ 607 (M^++1)
142				 ESI+ 607 (M^++1)

Table 25

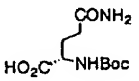
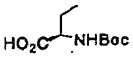
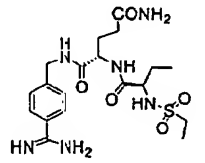
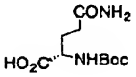
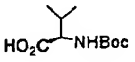
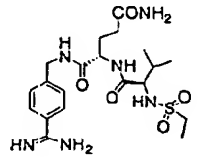
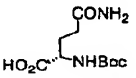
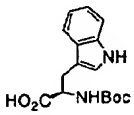
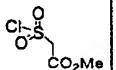
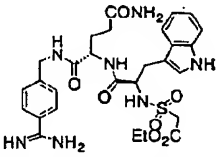
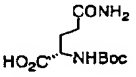
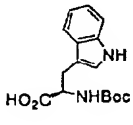
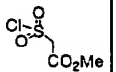
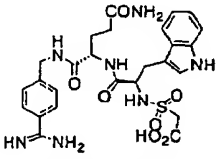
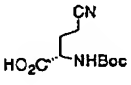
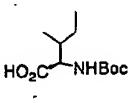
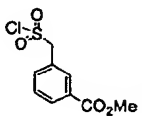
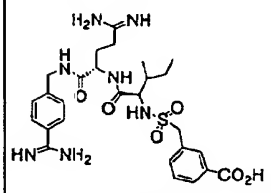
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
143				 ESI+ 455 (M^++1)
144				 ESI+ 469 (M^++1)
145				 ESI+ 614 (M^++1)
146				 ESI+ 586 (M^++1)
147				 ESI+ 588 (M^++1)

Table 26

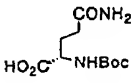
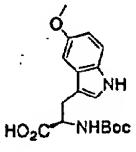
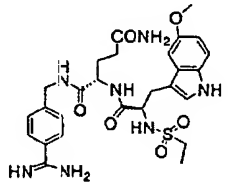
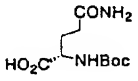
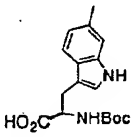
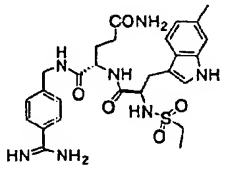
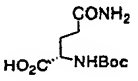
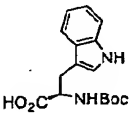
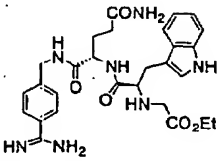
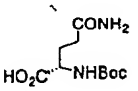
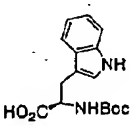
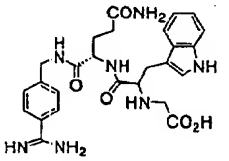
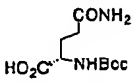
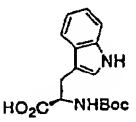
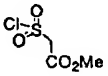
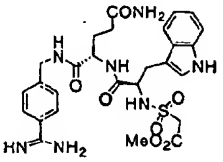
Example	Reagent 2	Reagent 5	Reagent 8	Structure MS
148				 ESI+ 586 (M^++1)
149				 ESI+ 570 (M^++1)
150				 ESI+ 550 (M^++1)
151				 ESI+ 522 (M^++1)
152				 ESI+ 600 (M^++1)

Table 27

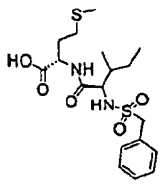
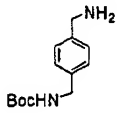
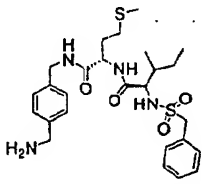
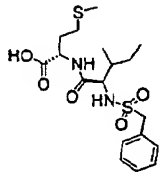
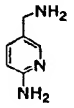
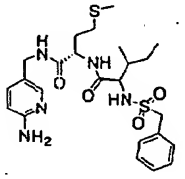
Example	Intermediate 17	Reagent 18	Structure MS
153			 ESI+ 535 (M^++1)
154			 ESI- 522 (M^++1)

Table 28

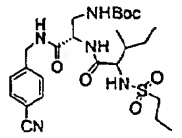
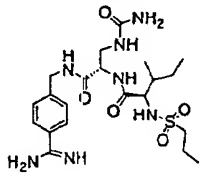
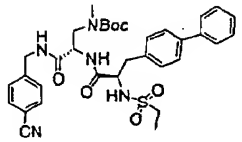
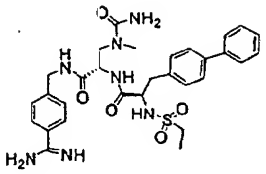
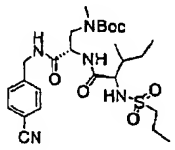
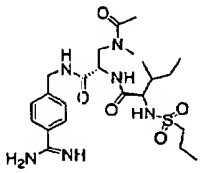
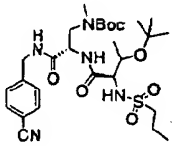
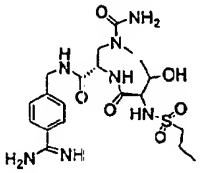
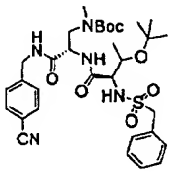
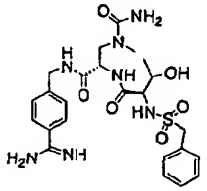
Example	Intermediate 9	Reagent 22	Structure MS
155		KNCO	 ESI+ 498 (M^++1)
156		KNCO	 ESI+ 608 (M^++1)
157		CH3COCl	 ESI+ 511 (M^++1)
158		KNCO	 ESI+ 500 (M^++1)
159		KNCO	 FAEI+ 548 (M^++1)

Table 29

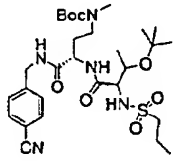
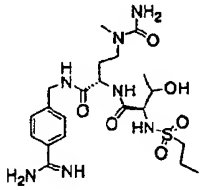
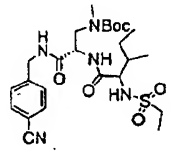
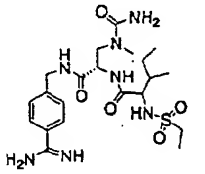
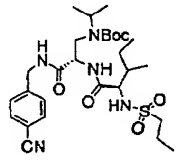
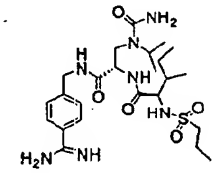
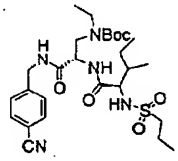
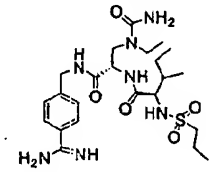
Example	Intermediate 9	Reagent 22	Structure MS
160		KNCO	 ESI+ 514 (M^++1)
161		KNCO	 ESI+ 498 (M^++1)
162		KNCO	 ESI+ 540 (M^++1)
163		KNCO	 ESI+ 526 (M^++1)

Table 30

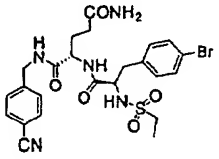
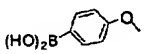
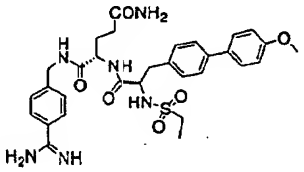
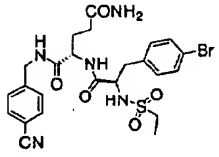
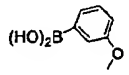
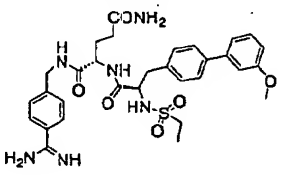
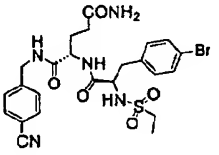
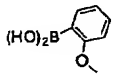
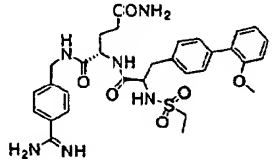
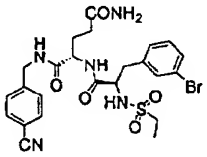
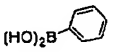
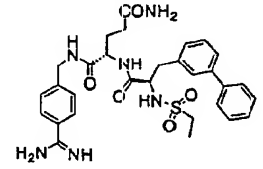
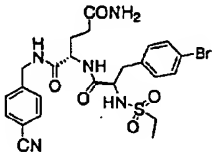
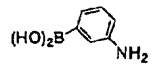
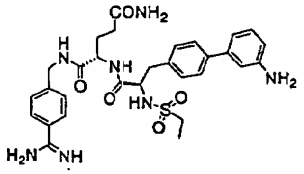
Example	Intermediate 34	Reagent 35	Structure MS
164			 ESI+ 623 (M^++1)
165			 ESI+ 623 (M^++1)
166			 ESI+ 623 (M^++1)
167			 ESI+ 593 (M^++1)
168			 ESI+ 608 (M^++1)

Table 31

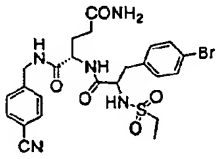
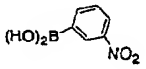
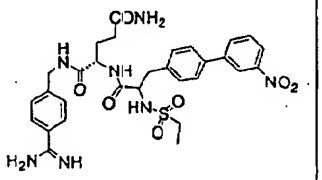
Example	Intermediate 34	Reagent 35	Structure MS
169			 ESI+ 638 (M^++1)

Table 32

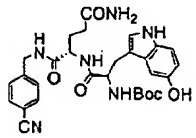
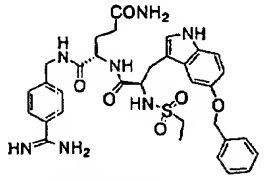
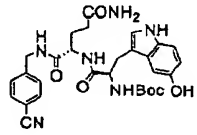
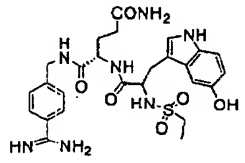
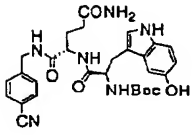
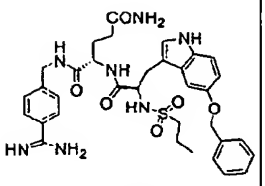
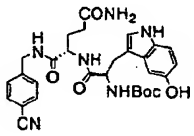
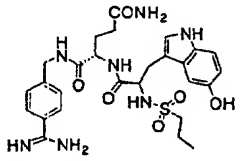
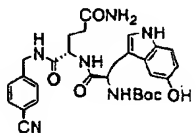
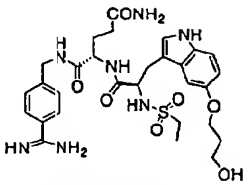
Example	Intermediate 38	Reagent 39	Reagent 8	Structure MS
170				 ESI+ 662 (M^++1)
171				 ESI+ 572 (M^++1)
172				 ESI+ 676 (M^++1)
173				 ESI+ 586 (M^++1)
174				 ESI+ 629 (M^++1)

Table 33

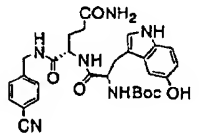
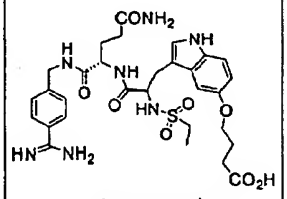
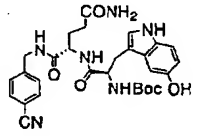
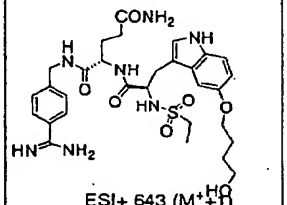
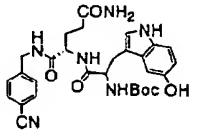
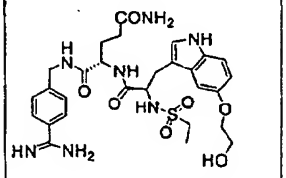
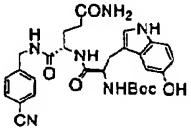
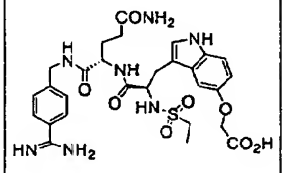
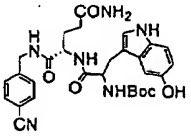
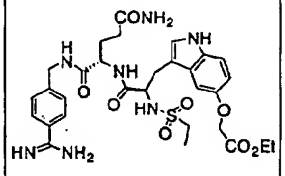
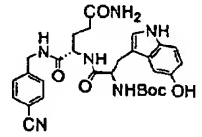
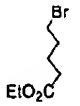
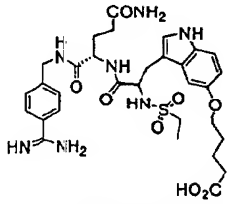
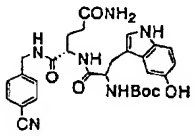
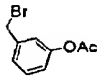
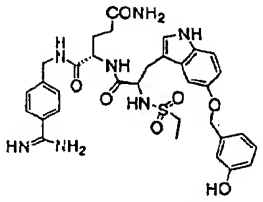
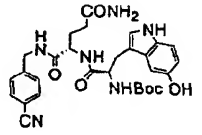
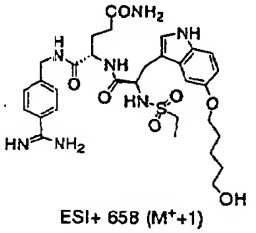
Example	Intermediate 38	Reagent 39	Reagent 8	Structure MS
175				 ESI+ 657 (M^++1)
176				 ESI+ 643 (M^++1)
177				 ESI+ 615 (M^++1)
178				 ESI+ 630 (M^++1)
179				 ESI+ 658 (M^++1)

Table 34

Example	Intermediate 38	Reagent 39	Reagent 8	Structure MS
180				 ESI+ 671 (M^++1)
181				 ESI+ 678 (M^++1)
182				 ESI+ 658 (M^++1)

Example 183

[Expression and purification of human factor VIIa]

[0189] Human factor VII cDNA was obtained from a human liver cDNA library (CLONTECH) by PCR. The primer sequences used are as follows:

GTCTGGATCCACCATGGTCTCCCAGGCCCTCAG

TGTTGAATTCTACTAGGGAAATGGGGCTCGCA.

[0190] The human factor VII gene was integrated into a Double One expression vector (IDEC), subcloned and digested with the restriction enzyme SspI. The linearized fragment was then introduced into the CHO cell line DG44 by electroporation to create human factor VII-expressing transformants. The transformants were then grown in the presence of 5 nM methotrexate (Sigma) for gene amplification. The resulting methotrexate-resistant human factor VII-expression transformants were further grown in a CHO-S-SFMII medium (GIBCO BRL) supplemented with 5 nmol/L methotrexate and 0.5 μg/ml vitamin K (Sigma) to express human factor VII.

[0191] The culture supernatant of human factor VII-expressing CHO transformants was concentrated through a hollow fiber dialyzer (PAN-130F, Asahi Medical Co., Ltd.) and supplemented with benzamidine at a final concentration of 5 mM for frozen storage. This frozen-stored culture supernatant was used, as appropriate, in purifying human factor VIIa. For purification, reference was made to Methods Enzymol., vol. 80, pages 228-237, 1981 and Biochemistry, vol. 27, pages 7785-7793, 1988. The concentrated culture supernatant was diluted 10-fold in 20 mM Tris-HCl buffer (pH 8.0) containing 5 mM benzamidine and 5 mM EDTA, and then applied to a Q Sepharose Fast Flow column equilibrated with the same buffer. Proteins adsorbed to the column were eluted with a stepwise gradient of NaCl (0.1, 0.2, 0.3 M) in the same buffer. The 0.3 M NaCl fractions containing human factor VII were concentrated by ultrafiltration, diluted 10-fold in 20 mM Tris-HCl buffer (pH 8.0) containing 5 mM benzamidine and 5 mM EDTA, and then applied to a Q Sepharose Fast Flow column equilibrated with the same buffer. After washing with the same buffer, human factor VII was eluted from the column with a linear $CaCl_2$ gradient up to 50 mM. The resulting fractions were analyzed by SDS/PAGE to collect human factor VII-containing fractions, which were then allowed to stand at room temperature for 2 days to facilitate self-digestion for activation into human factor VIIa. The reaction mixture was diluted 10-fold in 20 mM Tris-HCl buffer (pH 7.0) and then applied to a Q Sepharose Fast Flow column equilibrated with the same buffer. Human factor VIIa was eluted with a linear NaCl gradient of 150 to 350 mM in the same buffer. The resulting fractions were analyzed by SDS/PAGE to collect human factor VIIa-containing fractions, thus giving a purified human VIIa fraction.

Example 184

[Expression and purification of human soluble tissue factor]

[0192] A gene fragment encoding human soluble tissue factor (amino acids 1-218) was inserted downstream of the tac promoter and the M13 signal peptide sequence to create a secretory expression vector, which was then transformed into *E. coli* JM109 cells. The resulting transformants were grown to express human soluble tissue factor into the culture supernatant.

[0193] Purification was performed as described in Biochemistry, vol. 31, pages 3998-4003, 1992, with some modifications. The culture supernatant was concentrated by ultrafiltration and then treated with 65% saturated ammonium sulfate to precipitate the protein of interest. The precipitated product was collected by centrifugation (18000 g, 10 minutes), dissolved in PBS and then dialyzed against 25 mM acetate buffer (pH 5.2). The dialyzed solution was centrifuged (8000 g, 20 minutes) to remove insoluble products and the resulting supernatant was applied to an SP Sepharose Fast Flow column equilibrated with 25 mM acetate buffer (pH 5.2). Human soluble tissue factor was eluted from the column with a linear NaCl gradient up to 500 mM in the same buffer. The resulting fractions were analyzed by SDS/PAGE to collect fractions containing human soluble tissue factor, followed by dialysis against 25 mM Tris-HCl buffer (pH 7.5). The dialyzed fractions were applied to a Q Sepharose Fast Flow column equilibrated with 25 mM Tris-HCl buffer (pH 7.5) and human soluble tissue factor was eluted from the column with a linear NaCl gradient up to 500 mM in the same buffer, thus giving a purified human soluble tissue factor fraction.

Example 185

[Preparation of a human factor VIIa/human soluble tissue factor seed crystal]

[0194] As described in Proteins, vol. 22, pages 419-425, 1995, crystallization was performed on a complex between human factor VIIa and human soluble tissue factor, irreversibly inhibited with D-Phe-Phe-Arg chloromethylketone. This crystal is necessary as a seed crystal for crystallization of a complex between reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor. The purified human factor VIIa was mixed with a 10-fold molar excess of D-Phe-Phe-Arg chloromethylketone (BACHEM) and allowed to stand at 4°C for 3 hours. To this mixture, an excess amount of the purified human soluble tissue factor was added and allowed to stand at 37°C for 30 minutes, followed by ultrafiltration for concentration. The concentrated fraction was applied to a gel filtration column (Superdex 75) equilibrated with 50 mM Tris-HCl buffer (pH 7.5) containing 5 mM $CaCl_2$ and 100 mM NaCl, and then eluted with the same buffer to give a purified fraction of the human factor VIIa/human soluble tissue factor complex irreversibly inhibited with D-Phe-Phe-Arg chloromethylketone. This fraction was concentrated by ultrafiltration for crystallization to prepare a sample with a protein concentration of 10 mg/ml in 50 mM Tris-HCl buffer (pH 7.5), 100 mM NaCl and 5 mM $CaCl_2$. This sample was then allowed to stand at a temperature of 20°C using hanging drop vapor diffusion methods under reservoir conditions of 100 mM sodium cacodylate buffer (pH 5.0), 24% PEG40 and 5 mM $CaCl_2$, yielding a large amount of needle crystal.

Example 186

[Preparation of a human factor VIIa/human soluble tissue factor sample for crystallization]

[0195] After addition of 1/10 volumes of 1M benzamidine, the purified human factor VIIa was mixed with a molar excess of the purified human soluble tissue factor. This mixture was concentrated by ultrafiltration and then applied to a gel filtration column (Superdex 75) equilibrated with 50 mM Tris-HCl buffer (pH 7.5) containing 5 mM $CaCl_2$ and 100 mM NaCl. A human factor VIIa/human soluble tissue factor complex was eluted from the column with the same buffer to give a purified fraction of the human factor VIIa/human soluble tissue factor complex.

Example 187

[Crystallization of a complex between a low-molecular weight reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor]

[0196] The purified human factor VIIa/human soluble tissue factor complex was mixed with Compound (1) or (2) and then concentrated by ultrafiltration for crystallization to prepare a sample with a protein concentration of 12-13 mg/ml in 50 mM Tris-HCl buffer (pH 7.5), 100 mM NaCl and 5mM $CaCl_2$. Compounds (1) and (2) were used at the concentrations indicated in Table 35.

Table 35

	Compound (1)	Compound (2)
Concentration	0.5 mM	< 0.5 mM

[0197] Since spontaneous crystallization will not occur for a complex between a low-molecular weight reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor, it is necessary to add a seed crystal during crystallization. The seed crystal was prepared as follows. In a solution of 100 mM sodium cacodylate buffer (pH 5.0), 9% PEG4000 and 5mM $CaCl_2$, the crystal of the human factor VIIa/human soluble tissue factor complex irreversibly inhibited with D-Phe-Phe-Arg chloromethylketone was crushed with a homogenizer and then diluted to prepare a series of 10-fold dilutions from 10^{-1} to 10^{-6}. Likewise, a crystal of a complex between a low-molecular weight reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor was also available as a seed crystal.

[0198] Crystallization was performed by hanging drop vapor diffusion methods at a temperature of 25°C under reservoir conditions of 100 mM sodium cacodylate buffer (pH 5.0), 6% to 7.5% PEG4000, 5 mM $CaCl_2$ and 5% glycerol. The complex sample prepared from the low-molecular weight reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor was mixed with the reservoir and the seed dilutions at a ratio of 1.5 μl:1.5 μl:0.5 μl (sample:reservoir:seed) to prepare a crystallization drop. About a month later, long rod crystals (maximum size: about 1.0 mm long × 0.05 mm diameter) were obtained for the complex between the low-molecular weight reversible inhibitor and human factor VIIa/human soluble tissue factor.

Example 188

[Measurement of X-ray diffraction data]

(A) Crystal of the complex between Compound (1) and human factor VIIa/human soluble tissue factor

[0199] The crystal was soaked in 100 mM sodium cacodylate buffer (pH 5.0), 9% PEG40 and 5mM $CaCl_2$ with a 5% stepwise gradient of glycerol from 10% up to 30%. This crystal together with its surrounding solution was picked by a nylon loop (cryo-loop, Hampton research) and frozen in a nitrogen stream at -170°C. The crystal was maintained in a nitrogen stream at -170°C during measurement. X-ray diffraction data were collected using an R-axis IV imaging plate detector (Rigaku) under CuKα radiation from a rotating anode X-ray generator with a fine focus filament (Ultrax18, Rigaku) at 44 kV × 100 mA through OSMIC X-ray focusing mirrors (Rigaku). The DENZO/SCALEPACK program (Mac Science) was used for cell parameter and crystal orientation determination, diffraction spot indexing, as well as diffraction data processing, thereby obtaining diffraction intensity data up to 2.2 Å resolution. This crystal was found to be isomorphous to the Protein Data Bank complex of human factor VIIa/human soluble tissue factor, irreversibly inhibited with D-Phe-Phe-Arg chloromethylketone (PDB code: 1DAN). This crystal had space group $P2_12_12_1$ with unit cell parameters a = 71.40 Å, b = 82.22 Å, c = 123.47 Å, α = 90.0°, β = 90.0° and γ = 90.0°.

(B) Crystal of the complex between Compound (2) and human factor VIIa/human soluble tissue factor

[0200] The crystal was soaked in 100 mM sodium cacodylate buffer (pH 5.0), 9% PEG4000 and 5mM $CaCl_2$ with a 5% stepwise gradient of glycerol from 10% up to 30%. This crystal together with its surrounding solution was picked by a nylon loop (cryo-loop, Hampton research) and frozen in a nitrogen stream at -170°C. The crystal was maintained in a nitrogen stream at -170°C during measurement. X-ray diffraction data were collected using an R-axis IV imaging plate detector (Rigaku) under CuKα radiation from a rotating anode X-ray generator with a fine focus filament (Ultrax18 Rigaku) at 40 kV × 100 mA through Yale mirrors (Rigaku). The DENZO/SCALEPACK program (Mac Science) was used for cell parameter and crystal orientation determination, diffraction spot indexing, as well as diffraction data processing, thereby obtaining diffraction intensity data up to 2.2 Å resolution. This crystal was found to be isomorphous to the Protein Data Bank complex of human factor VIIa/human soluble tissue factor, irreversibly inhibited with D-Phe-Phe-Arg chloromethylketone (PDB code: 1DAN). This crystal had space group $P2_12_12_1$ with unit cell parameters a = 71.28 Å, b = 82.32 Å, c = 123.38 Å, α = 90.0°, β = 90.0° and γ = 90.0°.

Example 189

[Structure Analysis]

(A) Crystal of the complex between Compound (1) and human factor YIIa/human soluble tissue factor

[0201] Water molecules, and D-Phe-Phe-Arg chloromethylketone were removed from the coordinate data of the factor VIIa/tissue factor complex irreversibly inhibited with D-Phe-Phe-Arg chloromethylketone (PDB code: 1DAN) in the Protein Data Bank to create an initial model, followed by structure refinement using the CNX2000.1 program (Accerlys Inc). After rigid body refinement and energy minimization refinement, a Fourier map was calculated using coefficients 2Fo-Fc and Fo-Fc, where Fo was the structure factor observed experimentally and Fc was the structure factor calculated from the refined model. The map was then displayed on QUANTA to give a continuous electron density peak around the catalytic active center of factor VIIa. An atomic model for Compound (1) was fitted to this electron density peak, followed by several rounds of refinement by simulated annealing and energy minimization. The locations of water molecules were then determined based on the Fourier map with coefficients 2Fo-Fc and Fo-Fc, followed by simulated annealing refinement and energy minimization refinement. This procedure was repeated to give the final structure coordinates. The refined parameters were xyz coordinates and an isotropic temperature factor for each atom. The occupancy was set to 1.0 for each atom. The final structure contains cordinates of 5142 atoms (including 4688 protein atoms, 9 ion atoms, 404 water atoms and 41 inhibitor atoms), giving a reduction of crystallographic R factor to 22.59% for the 30.0-2.2 Å resolution data (34775 reflections). Meanwhile, the Free R value was 26.72% for 2627 reflections.

(B) Crystal of the complex between Compound (2) and human factor VIIa/human soluble tissue factor

[0202] Water molecules and D-Phe-Phe-Arg chloromethylketone were removed from the coordinate data of the factor VIIa/tissue factor complex irreversibly inhibited with D-Phe-Phe-Arg chloromethylketone (PDB code: 1DAN) in the

Protein Data Bank to create an initial model, followed by structure refinement using the CNX2000.1 program. After rigid body refinement and energy minimization refinement, a Fourier map was calculated using coefficients 2Fo-Fc and Fo-Fc, where Fo was the structure factor observed experimentally and Fc was the structure factor calculated from the refined model. The map was then displayed on QUANTA to give a continuous electron density peak around the catalytic active center of factor VIIa. An atomic model for Compound (2) was fitted to this electron density peak, followed by several rounds of refinement by simulated annealing and energy minimization. The locations of water molecules were then determined based on the Fourier map with coefficients 2Fo-Fc and Fo-Fc, followed by simulated annealing refinement and energy minimization refinement. This procedure was repeated to give the final structure coordinates. The refined parameters were xyz coordinates and an isotropic temperature factor for each atom. The occupancy was set to 1.0 for each atom. The final structure contains cordinates of 5193 atoms (including 4688 protein atoms, 9 ion atoms, 454 water atoms and 42 inhibitor atoms), giving a reduction of crystallographic R factor to 21.13% for the 30.0-2.2 Å resolution data (33708 reflections). Meanwhile, the Free R value was 25.08% for 2530 reflections.

Example 190

[Structure coordinates]

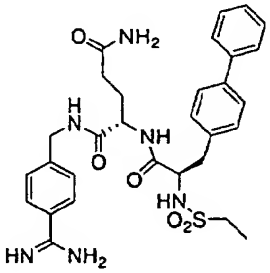
(A) Crystal structure coordinates of the complex between Compound (1) and human factor VIIa/human soluble tissue factor

[0203] The coordinates of all atoms were shown in PDB format in Table 36 (found at the end of the specification).

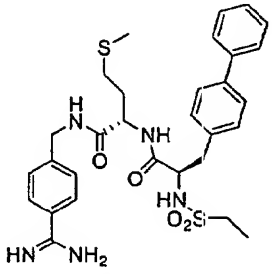
(B) Crystal structure coordinates of the complex between Compound (2) and human factor VIIa/human soluble tissue factor

[0204] The coordinates of Compound (2) and amino acid residues within 10 Å of Compound (2) were shown in PDB format in Table 37 (found at the end of the specification).

Table 38 Relationship between S2 site-binding moiety and human factor VIIa specificity



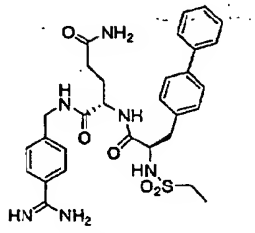
(2)
Example 65



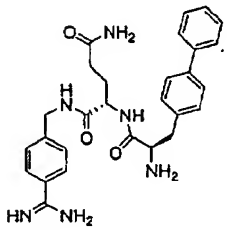
(3)
Example 67

Compound	Example	IC50 Factor VIIa (nM)	IC50 Thrombin (nM)	Thrombin selectivity
(2)	65	93	9415	101
(3)	67	341	2275	7

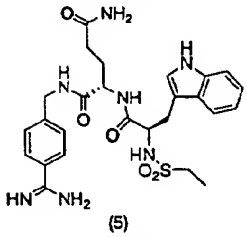
Table 39 Relationship between S1 subsite-binding moiety and human factor VIIa specificity



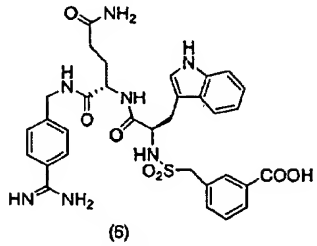
(2)
Example 65



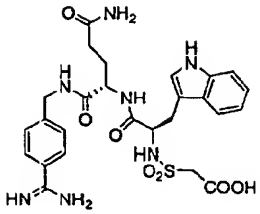
(4)
Example 66



(5)
Example 5



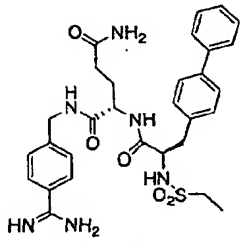
(6)
Example 7



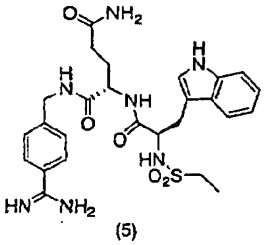
(1)
Example 146

Compound	Example	IC50 Factor VIIa (nM)	IC50 Thrombin (nM)	Thrombin selectivity
(2)	65	93	9415	101
(4)	66	2945	59051	20
(5)	5	62	5880	95
(6)	7	37	17870	483
(1)	146	153	80175	524

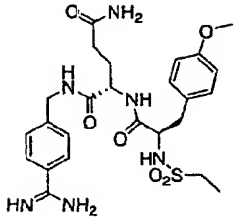
Table 40 Relationship between S4 site-binding moiety and human factor VIIa specificity



(2)
Example 65



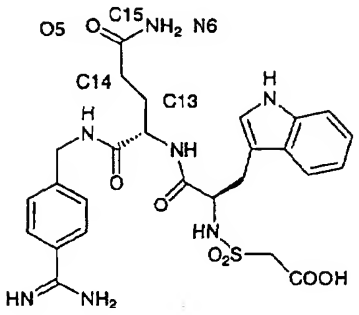
(5)
Example 5



(7)
Example 73

Compound	Example	IC50 Factor VIIa (nM)	IC50 Thrombin (nM)	Thrombin selectivity
(2)	65	93	9415	101
(5)	5	62	5880	95
(7)	73	81	397	5

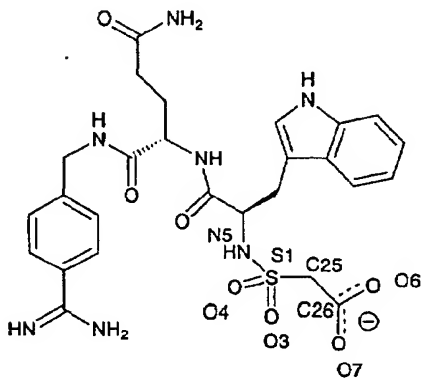
Table 41 Hydrogen bonding between Compound (1) and human factor VIIa S2 site



Hydrogen bonding

Inhibitor	Factor VIIa	Distance
N6	Asp60_OD2	3.0 Å
N6	Tyr94_OH	3.0 Å
N6	Thr98_O	2.8 Å
O5	Asp60_OD2	3.2 Å

Table 42 Hydrogen and ionic bonding between Compound (1) and human factor VIIa S1 subsite



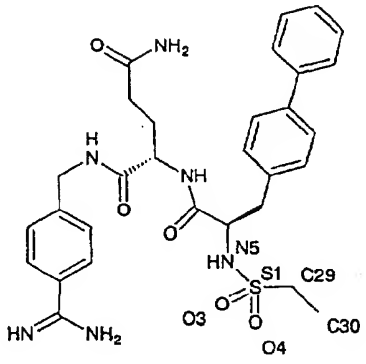
Hydrogen bonding

Inhibitor	Factor VIIa	Distance
N5	Gly216_O	2.9 Å
O4	Gly219_N	2.8 Å

Ionic bonding

Inhibitor	Factor VIIa	Distance
O7	Lys192_NZ	4.2 Å

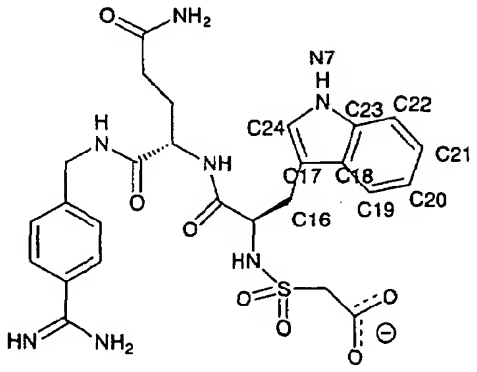
Table 43 Hydrogen bonding between Compound (2) and human factor VIIa S1 subsite



Hydrogen bonding

Inhibitor	Factor VIIa	Distance
N5	Gly216_O	2.8 Å
O3	Gly219_N	2.8 Å
O4	Lys192_NZ	3.2 Å

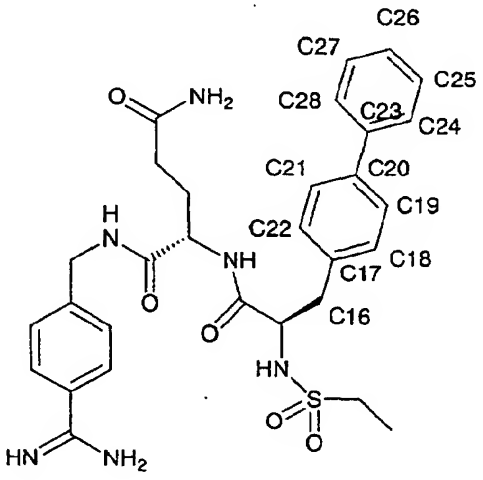
Table 44 Van der Waals interaction between Compound (1) and human factor VIIa S4 site



Ligand atom	Factor VIIa	Minimum distance	Factor VIIa	Minimum distance	Factor VIIa	Minimum distance
C16	Pro170I	3.9 Å				
C17	Pro170I	3.7 Å				
C18	Pro170I	3.4 Å				
C19	Pro170I	3.5 Å				
C20	Gln217	3.8 Å	Val170E	4.2 Å	Ser170H	4.1 Å
C20	Pro170I	4.0 Å				
C21	Val_170E	4.0 Å	Asp170G	4.2 Å	Ser170H	3.8 Å
C22	Asp170G	3.5 Å	Ser170H	4.1 Å		
C23	Asp170G	3.8 Å	Pro170I	3.8 Å		
C24	Pro170I	4.1 Å				
N7	Asp170G	4.0 Å				

* The above table exclusively shows ligand atoms located within a minimum distance of 4.2 Å from amino acid residues in human factor VIIa.

Table 45 Van der Waals interaction between Compound (2) and human factor VIIa S4 site



Ligand atom	Factor VIIa	Minimum distance	Factor VIIa	Minimum distance	Factor VIIa	Minimum distance
C16	Trp215	3.9 Å	Gly216	4.2 Å	Pro170I	4.0 Å
C17	Pro170I	3.6 Å				
C18	Pro170I	3.6 Å	Trp215	4.2 Å	Gln217	4.2 Å
C19	Ser170H	3.8 Å	Pro170I	3.6 Å	Gln217	3.9 Å
C20	Ser170H	3.9 Å	Pro170I	3.7 Å		
C21	Pro170I	3.7 Å				
C22	Pro170I	3.7 Å				
C23	Ser170H	3.7 Å				
C24	Ser170H	4.2 Å	Gln217	3.9 Å		
C25	Gln217	4.2 Å				
C26	Gly170F	4.2 Å				
C27	Asp170G	3.9 Å	Ser170H	3.9 Å		
C28	Asp170G	3.8 Å	Ser170H	3.6 Å		

* The above table exclusively shows ligand atoms located within a minimum distance of 4.2 Å from amino acid residues in human factor VIIa.

Test Example: Biological activity test

Method

1. Assay for FVIIa-inhibiting activity

[0205] The assay was carried out with 96-well microplates (Falcon, No. 3072) at room temperature.

[0206] A 10 vol% DMSO solution of a test compound (20 μL) was mixed with 40 μL Thromborel®S (50 mg/mL, Dade Behring, GTS-200A), 20 μL Spectrozyme®fVIIa (5 mmol/L, American Diagnostica Inc., #217L), 20 μL Tris buffer (500 mmol/L Tris/HCl, pH 7.5, 1500 mmol/L NaCl, 50 mmol/L $CaCl_2$) and 80 μL distilled water, followed by stirring. The reaction was initiated by addition of 20 μL FVIIa (20 nmol/L, Enzyme Research Laboratories, HF VIIa) and then monitored over time for absorbance at 405 nm using a microplate reader (Biorad, Model 3550) to determine the initial velocity of the reaction for each test compound. The initial reaction velocity was set to 100% in the case of adding 10 vol% DMSO alone, instead of a test compound. A concentration-reaction curve was prepared for FVIIa-inhibiting activity of each test compound to calculate a concentration at which the compound causes 50% inhibition of initial reaction velocity. This concentration was defined as an IC50 value.

2. Assay for thrombin-inhibiting activity

[0207] The assay was carried out with 96-well microplates (Falcon, No. 3072) at room temperature.

[0208] A 10 vol% DMSO solution of a test compound (20 μL) was mixed with 40 μL Tris buffer (200 mmol/L Tris/HCl, pH 8.0), 20 μL NaCl solution (1 mol/L), 20 μL FVR-pNa (2 mmol/L, SIGMA, B 7632) and 80 μL distilled water, followed by stirring. The reaction was initiated by addition of 20 μL human thrombin (5 U/mL, SIGMA, T 1063) and then monitored over time for absorbance at 405 nm using a microplate reader (Biorad, Model 3550) to determine the initial velocity of the reaction for each test compound. The same procedure as shown in assay for FVIIa-inhibiting activity was repeated to calculate an IC50 value for each test compound.

Result

[0209] The results obtained are shown in Table 46 below.

Table 46

Example No.	IC50 Factor VIIa (nM)	IC50 Thrombin (nM)
5	62	5880
7	37	17870
65	93	9415
81	177	5691
82	131	12544
170	37	9422
22	39	17544
146	153	80175
148	65	8325
83	55	14374

INDUSTRIAL APPLICABILITY

[0210] The compound of the present invention can have an excellent inhibitory activity against FVIIa or a selective inhibitory activity against extrinsic blood coagulation. This suggests that the compound of the present invention is expected to have pharmaceutical utility such as an antithrombotic agent with higher safety and fewer side effects (e. g., hemorrhage tendency). In particular, it is expected to have prophylactic or therapeutic utility for pathological conditions associated with the extrinsic coagulation pathway. More specifically, it is expected to be effective as a therapeutic or prophylactic agent for chronic thrombosis (e.g., postoperative deep vein thrombosis, post-PTCA restenosis, chronic DIC). cardioembolic strokes, cardiac infarction, cerebral infarction, etc.

[0211] In addition, it is not only possible to provide a crystal which can be used for X-ray crystal structure analysis with the aim of three-dimensional structure analysis of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, but it is also possible to computationally design a low-molecular weight reversible factor VIIa inhibitor using X-ray crystal structure analysis data. Therefore, such a design procedure enables the development of a low-molecular weight reversible factor VIIa inhibitor.

Table 36 Coordinate data of the complex between Compound (1) and human factor VIIa/soluble tissue factor (all data)

CRYST1	71.400	82.220	123.470	90.00	90.00	90.00	P212121					
ATOM	1	N	ALA	L	1	43.006	30.236	87.010	1.00	26.90	L	N
ATOM	2	CA	ALA	L	1	44.063	31.220	87.381	1.00	27.37	L	C
ATOM	3	C	ALA	L	1	44.489	30.945	88.817	1.00	28.56	L	C
ATOM	4	O	ALA	L	1	43.801	30.238	89.541	1.00	27.63	L	O
ATOM	5	CB	ALA	L	1	43.527	32.638	87.252	1.00	27.26	L	C
ATOM	6	N	ASN	L	2	45.618	31.505	89.233	1.00	29.16	L	N
ATOM	7	CA	ASN	L	2	46.105	31.273	90.585	1.00	29.83	L	C
ATOM	8	C	ASN	L	2	46.263	32.541	91.402	1.00	30.42	L	C
ATOM	9	O	ASN	L	2	46.985	33.456	91.018	1.00	32.56	L	O
ATOM	10	CB	ASN	L	2	47.444	30.533	90.546	1.00	27.10	L	C
ATOM	11	CG	ASN	L	2	47.320	29.133	89.989	1.00	27.19	L	C
ATOM	12	OD1	ASN	L	2	46.579	28.312	90.519	1.00	26.29	L	O
ATOM	13	ND2	ASN	L	2	48.049	28.851	88.917	1.00	27.22	L	N
ATOM	14	N	ALA	L	3	45.565	32.592	92.528	1.00	31.86	L	N
ATOM	15	CA	ALA	L	3	45.652	33.724	93.438	1.00	31.70	L	C
ATOM	16	C	ALA	L	3	46.428	33.192	94.641	1.00	32.24	L	C
ATOM	17	O	ALA	L	3	46.627	31.980	94.764	1.00	31.48	L	O
ATOM	18	CB	ALA	L	3	44.266	34.179	93.853	1.00	31.84	L	C
ATOM	19	N	PHE	L	4	46.864	34.085	95.524	1.00	32.19	L	N
ATOM	20	CA	PHE	L	4	47.636	33.676	96.697	1.00	31.55	L	C
ATOM	21	C	PHE	L	4	46.917	32.656	97.574	1.00	29.19	L	C
ATOM	22	O	PHE	L	4	45.798	32.893	98.025	1.00	30.82	L	O
ATOM	23	CB	PHE	L	4	48.003	34.897	97.548	1.00	33.52	L	C
ATOM	24	CG	PHE	L	4	48.900	34.574	98.715	1.00	35.99	L	C
ATOM	25	CD1	PHE	L	4	50.180	34.067	98.506	1.00	36.15	L	C
ATOM	26	CD2	PHE	L	4	48.464	34.768	100.021	1.00	36.15	L	C
ATOM	27	CE1	PHE	L	4	51.012	33.759	99.580	1.00	38.17	L	C
ATOM	28	CE2	PHE	L	4	49.289	34.464	101.103	1.00	38.45	L	C
ATOM	29	CZ	PHE	L	4	50.567	33.957	100.881	1.00	37.74	L	C
ATOM	30	N	LEU	L	5	47.569	31.519	97.796	1.00	27.82	L	N
ATOM	31	CA	LEU	L	5	47.044	30.442	98.640	1.00	26.01	L	C
ATOM	32	C	LEU	L	5	45.864	29.624	98.122	1.00	26.56	L	C
ATOM	33	O	LEU	L	5	45.505	28.619	98.730	1.00	27.40	L	O
ATOM	34	CB	LEU	L	5	46.682	30.985	100.027	1.00	24.14	L	C
ATOM	35	CG	LEU	L	5	47.816	31.543	100.891	1.00	24.48	L	C
ATOM	36	CD1	LEU	L	5	47.248	31.998	102.231	1.00	22.64	L	C
ATOM	37	CD2	LEU	L	5	48.886	30.479	101.102	1.00	21.31	L	C
ATOM	38	N	CGU	L	6	45.252	30.027	97.016	1.00	26.55	L	N
ATOM	39	CA	CGU	L	6	44.120	29.256	96.516	1.00	26.75	L	C
ATOM	40	CB	CGU	L	6	43.497	29.921	95.289	1.00	26.18	L	C
ATOM	41	CG	CGU	L	6	42.283	29.117	94.819	1.00	25.49	L	C
ATOM	42	CD1	CGU	L	6	42.608	28.386	93.520	1.00	23.72	L	C
ATOM	43	CD2	CGU	L	6	41.068	30.027	94.667	1.00	26.90	L	C
ATOM	44	OE1	CGU	L	6	43.364	28.939	92.739	1.00	19.08	L	O
ATOM	45	OE2	CGU	L	6	42.108	27.273	93.323	1.00	22.25	L	O
ATOM	46	OE3	CGU	L	6	40.524	30.434	95.688	1.00	27.43	L	O
ATOM	47	OE4	CGU	L	6	40.690	30.308	93.557	1.00	26.50	L	O

ATOM	48	C	CGU	L	6	44.499	27.819	96.178	1.00	25.52	L	C
ATOM	49	O	CGU	L	6	43.666	26.915	96.256	1.00	24.58	L	O
ATOM	50	N	CGU	L	7	45.760	27.607	95.813	1.00	24.67	L	N
ATOM	51	CA	CGU	L	7	46.245	26.273	95.478	1.00	24.21	L	C
ATOM	52	CB	CGU	L	7	47.622	26.392	94.817	1.00	23.05	L	C
ATOM	53	CG	CGU	L	7	47.330	27.007	93.446	1.00	25.83	L	C
ATOM	54	CD1	CGU	L	7	46.490	26.029	92.643	1.00	25.89	L	C
ATOM	55	CD2	CGU	L	7	48.590	27.400	92.679	1.00	27.73	L	C
ATOM	56	OE1	CGU	L	7	45.505	26.442	92.115	1.00	24.48	L	O
ATOM	57	OE2	CGU	L	7	46.845	24.866	92.591	1.00	23.44	L	O
ATOM	58	OE3	CGU	L	7	49.041	28.527	92.846	1.00	28.58	L	O
ATOM	59	OE4	CGU	L	7	49.090	26.585	91.922	1.00	28.37	L	O
ATOM	60	C	CGU	L	7	46.249	25.303	96.672	1.00	23.79	L	C
ATOM	61	O	CGU	L	7	46.558	24.120	96.529	1.00	25.13	L	O
ATOM	62	N	LEU	L	8	45.896	25.811	97.848	1.00	24.29	L	N
ATOM	63	CA	LEU	L	8	45.789	24.983	99.049	1.00	24.16	L	C
ATOM	64	C	LEU	L	8	44.458	24.235	98.963	1.00	25.54	L	C
ATOM	65	O	LEU	L	8	44.285	23.180	99.565	1.00	26.65	L	O
ATOM	66	CB	LEU	L	8	45.790	25.851	100.311	1.00	23.41	L	C
ATOM	67	CG	LEU	L	8	47.117	26.250	100.968	1.00	24.22	L	C
ATOM	68	CD1	LEU	L	8	48.042	26.938	99.969	1.00	19.80	L	C
ATOM	69	CD2	LEU	L	8	46.817	27.166	102.148	1.00	23.24	L	C
ATOM	70	N	ARG	L	9	43.520	24.798	98.203	1.00	27.13	L	N
ATOM	71	CA	ARG	L	9	42.198	24.213	98.027	1.00	27.75	L	C
ATOM	72	C	ARG	L	9	42.226	23.132	96.949	1.00	27.08	L	C
ATOM	73	O	ARG	L	9	42.930	23.255	95.948	1.00	27.06	L	O
ATOM	74	CB	ARG	L	9	41.192	25.300	97.625	1.00	29.68	L	C
ATOM	75	CG	ARG	L	9	41.292	26.593	98.427	1.00	33.48	L	C
ATOM	76	CD	ARG	L	9	40.264	27.619	97.964	1.00	34.05	L	C
ATOM	77	NE	ARG	L	9	38.914	27.246	98.370	1.00	37.69	L	N
ATOM	78	CZ	ARG	L	9	38.254	27.781	99.395	1.00	38.57	L	C
ATOM	79	NH1	ARG	L	9	38.806	28.734	100.136	1.00	38.38	L	N
ATOM	80	NH2	ARG	L	9	37.037	27.349	99.689	1.00	40.53	L	N
ATOM	81	N	PRO	L	10	41.465	22.050	97.144	1.00	27.28	L	N
ATOM	82	CA	PRO	L	10	41.446	20.985	96.137	1.00	27.55	L	C
ATOM	83	C	PRO	L	10	41.008	21.551	94.780	1.00	27.58	L	C
ATOM	84	O	PRO	L	10	40.388	22.615	94.713	1.00	27.34	L	O
ATOM	85	CB	PRO	L	10	40.433	19.999	96.708	1.00	29.14	L	C
ATOM	86	CG	PRO	L	10	40.613	20.160	98.191	1.00	27.86	L	C
ATOM	87	CD	PRO	L	10	40.686	21.665	98.333	1.00	28.70	L	C
ATOM	88	N	GLY	L	11	41.334	20.848	93.702	1.00	26.59	L	N
ATOM	89	CA	GLY	L	11	40.950	21.321	92.383	1.00	28.67	L	C
ATOM	90	C	GLY	L	11	39.445	21.370	92.164	1.00	29.12	L	C
ATOM	91	O	GLY	L	11	38.709	20.499	92.628	1.00	30.35	L	O
ATOM	92	N	SER	L	12	38.985	22.398	91.459	1.00	29.23	L	N
ATOM	93	CA	SER	L	12	37.567	22.560	91.159	1.00	29.12	L	C
ATOM	94	C	SER	L	12	37.393	23.085	89.740	1.00	29.51	L	C
ATOM	95	O	SER	L	12	37.797	24.206	89.425	1.00	28.38	L	O
ATOM	96	CB	SER	L	12	36.916	23.531	92.143	1.00	30.52	L	C
ATOM	97	OG	SER	L	12	35.555	23.749	91.803	1.00	31.56	L	O
ATOM	98	N	LEU	L	13	36.788	22.271	88.884	1.00	29.17	L	N
ATOM	99	CA	LEU	L	13	36.575	22.660	87.497	1.00	30.18	L	C
ATOM	100	C	LEU	L	13	35.779	23.953	87.383	1.00	30.11	L	C
ATOM	101	O	LEU	L	13	36.128	24.844	86.611	1.00	32.23	L	O
ATOM	102	CB	LEU	L	13	35.842	21.549	86.745	1.00	30.30	L	C
ATOM	103	CG	LEU	L	13	35.630	21.832	85.260	1.00	31.24	L	C

ATOM	104	CD1	LEU	L	13	36.982	21.877	84.558	1.00	29.56	L	C
ATOM	105	CD2	LEU	L	13	34.743	20.756	84.654	1.00	30.75	L	C
ATOM	106	N	CGU	L	14	34.703	24.051	88.153	1.00	29.30	L	N
ATOM	107	CA	CGU	L	14	33.851	25.230	88.130	1.00	29.52	L	C
ATOM	108	CB	CGU	L	14	32.668	25.027	89.072	1.00	31.22	L	C
ATOM	109	CG	CGU	L	14	31.651	26.161	89.091	1.00	35.34	L	C
ATOM	110	CD1	CGU	L	14	30.495	25.800	90.019	1.00	36.63	L	C
ATOM	111	CD2	CGU	L	14	31.135	26.407	87.679	1.00	36.12	L	C
ATOM	112	OE1	CGU	L	14	29.836	26.703	90.495	1.00	37.62	L	O
ATOM	113	OE2	CGU	L	14	30.285	24.609	90.254	1.00	40.38	L	O
ATOM	114	OE3	CGU	L	14	31.048	27.567	87.288	1.00	37.34	L	O
ATOM	115	OE4	CGU	L	14	30.838	25.432	86.992	1.00	37.27	L	O
ATOM	116	C	CGU	L	14	34.585	26.515	88.502	1.00	28.40	L	C
ATOM	117	O	CGU	L	14	34.616	27.463	87.725	1.00	28.45	L	O
ATOM	118	N	ARG	L	15	35.177	26.540	89.691	1.00	27.46	L	N
ATOM	119	CA	ARG	L	15	35.894	27.718	90.175	1.00	27.51	L	C
ATOM	120	C	ARG	L	15	37.132	28.064	89.356	1.00	27.23	L	C
ATOM	121	O	ARG	L	15	37.465	29.237	89.182	1.00	25.95	L	O
ATOM	122	CB	ARG	L	15	36.313	27.508	91.637	1.00	27.70	L	C
ATOM	123	CG	ARG	L	15	37.003	28.707	92.288	1.00	28.99	L	C
ATOM	124	CD	ARG	L	15	37.615	28.338	93.650	1.00	27.72	L	C
ATOM	125	NE	ARG	L	15	38.708	27.374	93.512	1.00	23.84	L	N
ATOM	126	CZ	ARG	L	15	38.726	26.161	94.058	1.00	24.64	L	C
ATOM	127	NH1	ARG	L	15	37.710	25.737	94.798	1.00	25.00	L	N
ATOM	128	NH2	ARG	L	15	39.759	25.358	93.848	1.00	23.56	L	N
ATOM	129	N	CGU	L	16	37.792	27.036	88.835	1.00	27.33	L	N
ATOM	130	CA	CGU	L	16	39.032	27.205	88.085	1.00	27.34	L	C
ATOM	131	CB	CGU	L	16	39.967	26.045	88.431	1.00	27.36	L	C
ATOM	132	CG	CGU	L	16	40.198	25.989	89.937	1.00	23.86	L	C
ATOM	133	CD1	CGU	L	16	40.616	27.379	90.373	1.00	24.51	L	C
ATOM	134	CD2	CGU	L	16	41.304	24.995	90.253	1.00	23.35	L	C
ATOM	135	OE1	CGU	L	16	41.440	27.927	89.699	1.00	27.27	L	O
ATOM	136	OE2	CGU	L	16	40.095	27.883	91.340	1.00	24.69	L	O
ATOM	137	OE3	CGU	L	16	42.407	25.416	90.385	1.00	20.19	L	O
ATOM	138	OE4	CGU	L	16	41.023	23.818	90.349	1.00	22.98	L	O
ATOM	139	C	CGU	L	16	38.982	27.363	86.574	1.00	29.25	L	C
ATOM	140	O	CGU	L	16	39.739	28.159	86.011	1.00	29.12	L	O
ATOM	141	N	CYS	L	17	38.113	26.607	85.913	1.00	29.27	L	N
ATOM	142	CA	CYS	L	17	38.020	26.672	84.460	1.00	30.58	L	C
ATOM	143	C	CYS	L	17	36.760	27.339	83.910	1.00	30.90	L	C
ATOM	144	O	CYS	L	17	36.767	27.841	82.789	1.00	31.41	L	O
ATOM	145	CB	CYS	L	17	38.143	25.268	83.870	1.00	29.03	L	C
ATOM	146	SG	CYS	L	17	39.683	24.375	84.273	1.00	29.62	L	S
ATOM	147	N	LYS	L	18	35.682	27.337	84.686	1.00	33.15	L	N
ATOM	148	CA	LYS	L	18	34.428	27.953	84.254	1.00	33.15	L	C
ATOM	149	C	LYS	L	18	34.376	29.423	84.649	1.00	33.16	L	C
ATOM	150	O	LYS	L	18	34.202	30.299	83.804	1.00	33.01	L	O
ATOM	151	CB	LYS	L	18	33.229	27.210	84.855	1.00	33.20	L	C
ATOM	152	CG	LYS	L	18	32.773	25.998	84.049	1.00	35.52	L	C
ATOM	153	CD	LYS	L	18	33.805	24.888	84.034	1.00	38.86	L	C
ATOM	154	CE	LYS	L	18	34.139	24.448	82.610	1.00	39.72	L	C
ATOM	155	NZ	LYS	L	18	32.971	23.879	81.874	1.00	40.07	L	N
ATOM	156	N	CGU	L	19	34.525	29.686	85.942	1.00	33.87	L	N
ATOM	157	CA	CGU	L	19	34.510	31.048	86.459	1.00	33.17	L	C
ATOM	158	CB	CGU	L	19	34.259	31.030	87.963	1.00	34.83	L	C
ATOM	159	CG	CGU	L	19	32.874	30.589	88.419	1.00	37.03	L	C

ATOM	160	CD1	CGU	L	19	31.834	31.593	87.934	1.00	37.84	L	C
ATOM	161	CD2	CGU	L	19	32.836	30.518	89.941	1.00	39.06	L	C
ATOM	162	OE1	CGU	L	19	30.658	31.307	88.057	1.00	36.43	L	O
ATOM	163	OE2	CGU	L	19	32.229	32.655	87.435	1.00	39.63	L	O
ATOM	164	OE3	CGU	L	19	32.692	29.414	90.470	1.00	38.92	L	O
ATOM	165	OE4	CGU	L	19	32.955	31.571	90.570	1.00	41.50	L	O
ATOM	166	C	CGU	L	19	35.826	31.771	86.182	1.00	32.60	L	C
ATOM	167	O	CGU	L	19	35.934	32.978	86.388	1.00	33.89	L	O
ATOM	168	N	CGU	L	20	36.824	31.030	85.714	1.00	31.95	L	N
ATOM	169	CA	CGU	L	20	38.128	31.607	85.422	1.00	30.77	L	C
ATOM	170	CB	CGU	L	20	39.045	31.487	86.634	1.00	28.99	L	C
ATOM	171	CG	CGU	L	20	38.620	31.952	88.020	1.00	30.59	L	C
ATOM	172	CD1	CGU	L	20	38.770	33.462	88.131	1.00	31.48	L	C
ATOM	173	CD2	CGU	L	20	39.521	31.281	89.047	1.00	30.25	L	C
ATOM	174	OE1	CGU	L	20	38.025	34.061	88.882	1.00	33.25	L	O
ATOM	175	OE2	CGU	L	20	39.634	34.004	87.461	1.00	33.62	L	O
ATOM	176	OE3	CGU	L	20	39.282	31.444	90.226	1.00	29.48	L	O
ATOM	177	OE4	CGU	L	20	40.453	30.598	88.629	1.00	30.41	L	O
ATOM	178	C	CGU	L	20	38.791	30.857	84.283	1.00	29.55	L	C
ATOM	179	O	CGU	L	20	38.328	29.796	83.875	1.00	29.94	L	O
ATOM	180	N	GLN	L	21	39.891	31.419	83.795	1.00	30.03	L	N
ATOM	181	CA	GLN	L	21	40.680	30.808	82.739	1.00	30.36	L	C
ATOM	182	C	GLN	L	21	41.690	29.913	83.454	1.00	29.74	L	C
ATOM	183	O	GLN	L	21	42.484	30.388	84.276	1.00	27.73	L	O
ATOM	184	CB	GLN	L	21	41.425	31.879	81.944	1.00	33.78	L	C
ATOM	185	CG	GLN	L	21	40.535	32.812	81.134	1.00	40.75	L	C
ATOM	186	CD	GLN	L	21	39.865	32.115	79.966	1.00	44.61	L	C
ATOM	187	OE1	GLN	L	21	39.029	31.228	80.150	1.00	48.21	L	O
ATOM	188	NE2	GLN	L	21	40.235	32.510	78.752	1.00	45.88	L	N
ATOM	189	N	CYS	L	22	41.659	28.621	83.159	1.00	27.02	L	N
ATOM	190	CA	CYS	L	22	42.584	27.704	83.798	1.00	26.53	L	C
ATOM	191	C	CYS	L	22	43.607	27.197	82.795	1.00	28.06	L	C
ATOM	192	O	CYS	L	22	43.285	26.959	81.630	1.00	29.00	L	O
ATOM	193	CB	CYS	L	22	41.824	26.529	84.417	1.00	26.03	L	C
ATOM	194	SG	CYS	L	22	41.127	25.347	83.224	1.00	24.58	L	S
ATOM	195	N	SER	L	23	44.846	27.044	83.251	1.00	28.01	L	N
ATOM	196	CA	SER	L	23	45.919	26.564	82.395	1.00	29.36	L	C
ATOM	197	C	SER	L	23	45.856	25.046	82.316	1.00	29.53	L	C
ATOM	198	O	SER	L	23	45.041	24.409	82.991	1.00	28.50	L	O
ATOM	199	CB	SER	L	23	47.278	26.991	82.954	1.00	30.24	L	C
ATOM	200	OG	SER	L	23	47.547	26.328	84.176	1.00	32.90	L	O
ATOM	201	N	PHE	L	24	46.729	24.471	81.496	1.00	28.75	L	N
ATOM	202	CA	PHE	L	24	46.774	23.030	81.325	1.00	28.22	L	C
ATOM	203	C	PHE	L	24	47.044	22.340	82.659	1.00	28.31	L	C
ATOM	204	O	PHE	L	24	46.373	21.370	83.019	1.00	26.88	L	O
ATOM	205	CB	PHE	L	24	47.871	22.644	80.328	1.00	27.99	L	C
ATOM	206	CG	PHE	L	24	47.906	21.179	80.019	1.00	27.32	L	C
ATOM	207	CD1	PHE	L	24	47.014	20.626	79.106	1.00	27.03	L	C
ATOM	208	CD2	PHE	L	24	48.791	20.338	80.684	1.00	27.00	L	C
ATOM	209	CE1	PHE	L	24	47.000	19.256	78.864	1.00	25.26	L	C
ATOM	210	CE2	PHE	L	24	48.784	18.964	80.449	1.00	25.45	L	C
ATOM	211	CZ	PHE	L	24	47.887	18.423	79.540	1.00	25.69	L	C
ATOM	212	N	CGU	L	25	48.031	22.850	83.388	1.00	27.44	L	N
ATOM	213	CA	CGU	L	25	48.405	22.282	84.673	1.00	28.71	L	C
ATOM	214	CB	CGU	L	25	49.570	23.068	85.262	1.00	33.43	L	C
ATOM	215	CG	CGU	L	25	50.357	22.364	86.358	1.00	38.45	L	C

ATOM	216	CD1	CGU	L	25	51.791	22.882	86.348	1.00	40.65	L	C
ATOM	217	CD2	CGU	L	25	50.357	20.859	86.100	1.00	40.80	L	C
ATOM	218	OE1	CGU	L	25	52.101	23.772	87.138	1.00	41.24	L	O
ATOM	219	OE2	CGU	L	25	52.571	22.386	85.537	1.00	43.46	L	O
ATOM	220	OE3	CGU	L	25	50.854	20.453	85.053	1.00	41.65	L	O
ATOM	221	OE4	CGU	L	25	49.853	20.120	86.950	1.00	42.95	L	O
ATOM	222	C	CGU	L	25	47.233	22.264	85.644	1.00	26.61	L	C
ATOM	223	O	CGU	L	25	46.958	21.246	86.271	1.00	25.98	L	O
ATOM	224	N	CGU	L	26	46.541	23.391	85.765	1.00	25.93	L	N
ATOM	225	CA	CGU	L	26	45.389	23.474	86.652	1.00	26.06	L	C
ATOM	226	CB	CGU	L	26	44.770	24.870	86.576	1.00	24.81	L	C
ATOM	227	CG	CGU	L	26	45.740	25.994	86.948	1.00	26.07	L	C
ATOM	228	CD1	CGU	L	26	46.302	25.752	88.351	1.00	26.84	L	C
ATOM	229	CD2	CGU	L	26	45.038	27.349	86.880	1.00	26.66	L	C
ATOM	230	OE1	CGU	L	26	45.548	25.374	89.218	1.00	24.86	L	O
ATOM	231	OE2	CGU	L	26	47.480	25.942	88.538	1.00	26.84	L	O
ATOM	232	OE3	CGU	L	26	44.976	27.925	85.801	1.00	28.65	L	O
ATOM	233	OE4	CGU	L	26	44.567	27.805	87.890	1.00	26.86	L	O
ATOM	234	C	CGU	L	26	44.360	22.416	86.254	1.00	26.09	L	C
ATOM	235	O	CGU	L	26	43.830	21.696	87.099	1.00	26.77	L	O
ATOM	236	N	ALA	L	27	44.090	22.319	84.957	1.00	26.92	L	N
ATOM	237	CA	ALA	L	27	43.139	21.341	84.449	1.00	26.84	L	C
ATOM	238	C	ALA	L	27	43.590	19.927	84.797	1.00	26.93	L	C
ATOM	239	O	ALA	L	27	42.775	19.085	85.171	1.00	27.45	L	O
ATOM	240	CB	ALA	L	27	42.999	21.486	82.938	1.00	24.94	L	C
ATOM	241	N	ARG	L	28	44.891	19.669	84.678	1.00	27.54	L	N
ATOM	242	CA	ARG	L	28	45.434	18.347	84.977	1.00	29.15	L	C
ATOM	243	C	ARG	L	28	45.275	17.976	86.451	1.00	29.86	L	C
ATOM	244	O	ARG	L	28	45.145	16.804	86.785	1.00	31.18	L	O
ATOM	245	CB	ARG	L	28	46.911	18.278	84.600	1.00	30.06	L	C
ATOM	246	CG	ARG	L	28	47.457	16.859	84.531	1.00	32.65	L	C
ATOM	247	CD	ARG	L	28	48.977	16.856	84.601	1.00	36.00	L	C
ATOM	248	NE	ARG	L	28	49.441	17.365	85.890	1.00	37.93	L	N
ATOM	249	CZ	ARG	L	28	49.284	16.735	87.053	1.00	38.70	L	C
ATOM	250	NH1	ARG	L	28	48.682	15.552	87.109	1.00	38.86	L	N
ATOM	251	NH2	ARG	L	28	49.706	17.308	88.171	1.00	39.29	L	N
ATOM	252	N	CGU	L	29	45.302	18.969	87.333	1.00	29.50	L	N
ATOM	253	CA	CGU	L	29	45.131	18.714	88.761	1.00	29.34	L	C
ATOM	254	CB	CGU	L	29	45.529	19.947	89.559	1.00	28.96	L	C
ATOM	255	CG	CGU	L	29	47.033	20.154	89.530	1.00	30.94	L	C
ATOM	256	CD1	CGU	L	29	47.709	19.275	90.575	1.00	33.97	L	C
ATOM	257	CD2	CGU	L	29	47.360	21.610	89.778	1.00	29.62	L	C
ATOM	258	OE1	CGU	L	29	48.900	19.048	90.442	1.00	37.46	L	O
ATOM	259	OE2	CGU	L	29	47.028	18.834	91.503	1.00	36.82	L	O
ATOM	260	OE3	CGU	L	29	48.486	21.975	89.603	1.00	27.06	L	O
ATOM	261	OE4	CGU	L	29	46.476	22.332	90.128	1.00	28.53	L	O
ATOM	262	C	CGU	L	29	43.688	18.343	89.077	1.00	28.66	L	C
ATOM	263	O	CGU	L	29	43.401	17.742	90.113	1.00	29.88	L	O
ATOM	264	N	ILE	L	30	42.783	18.717	88.181	1.00	27.56	L	N
ATOM	265	CA	ILE	L	30	41.371	18.408	88.340	1.00	27.41	L	C
ATOM	266	C	ILE	L	30	41.103	17.006	87.791	1.00	28.29	L	C
ATOM	267	O	ILE	L	30	40.605	16.138	88.503	1.00	28.57	L	O
ATOM	268	CB	ILE	L	30	40.492	19.428	87.570	1.00	26.20	L	C
ATOM	269	CG1	ILE	L	30	40.685	20.830	88.156	1.00	25.87	L	C
ATOM	270	CG2	ILE	L	30	39.035	19.014	87.626	1.00	23.37	L	C
ATOM	271	CD1	ILE	L	30	39.890	21.910	87.444	1.00	25.78	L	C

ATOM	272	N	PHE	L	31	41.454	16.794	86.525	1.00	28.80	L	N
ATOM	273	CA	PHE	L	31	41.237	15.512	85.855	1.00	32.23	L	C
ATOM	274	C	PHE	L	31	42.260	14.420	86.195	1.00	34.25	L	C
ATOM	275	O	PHE	L	31	41.958	13.230	86.097	1.00	34.78	L	O
ATOM	276	CB	PHE	L	31	41.188	15.739	84.341	1.00	30.23	L	C
ATOM	277	CG	PHE	L	31	40.039	16.608	83.900	1.00	28.90	L	C
ATOM	278	CD1	PHE	L	31	38.737	16.111	83.893	1.00	29.15	L	C
ATOM	279	CD2	PHE	L	31	40.254	17.926	83.512	1.00	25.49	L	C
ATOM	280	CE1	PHE	L	31	37.664	16.918	83.503	1.00	27.09	L	C
ATOM	281	CE2	PHE	L	31	39.194	18.740	83.123	1.00	25.64	L	C
ATOM	282	CZ	PHE	L	31	37.896	18.237	83.118	1.00	26.07	L	C
ATOM	283	N	LYS	L	32	43.463	14.832	86.586	1.00	36.51	L	N
ATOM	284	CA	LYS	L	32	44.544	13.919	86.967	1.00	39.51	L	C
ATOM	285	C	LYS	L	32	45.132	13.120	85.800	1.00	40.53	L	C
ATOM	286	O	LYS	L	32	46.265	13.362	85.386	1.00	41.25	L	O
ATOM	287	CB	LYS	L	32	44.064	12.958	88.064	1.00	40.66	L	C
ATOM	288	CG	LYS	L	32	43.132	13.599	89.088	1.00	43.75	L	C
ATOM	289	CD	LYS	L	32	43.294	13.002	90.473	1.00	45.44	L	C
ATOM	290	CE	LYS	L	32	44.566	13.514	91.136	1.00	48.55	L	C
ATOM	291	NZ	LYS	L	32	44.556	15.002	91.284	1.00	49.03	L	N
ATOM	292	N	ASP	L	33	44.366	12.167	85.278	1.00	41.87	L	N
ATOM	293	CA	ASP	L	33	44.811	11.343	84.161	1.00	43.56	L	C
ATOM	294	C	ASP	L	33	45.103	12.193	82.922	1.00	44.09	L	C
ATOM	295	O	ASP	L	33	44.322	13.073	82.562	1.00	44.53	L	O
ATOM	296	CB	ASP	L	33	43.747	10.290	83.849	1.00	45.31	L	C
ATOM	297	CG	ASP	L	33	44.088	9.458	82.635	1.00	47.36	L	C
ATOM	298	OD1	ASP	L	33	43.843	9.923	81.525	1.00	45.97	L	O
ATOM	299	OD2	ASP	L	33	44.606	8.347	82.809	1.00	49.11	L	O
ATOM	300	N	ALA	L	34	46.235	11.920	82.279	1.00	44.21	L	N
ATOM	301	CA	ALA	L	34	46.666	12.657	81.092	1.00	44.90	L	C
ATOM	302	C	ALA	L	34	45.679	12.572	79.932	1.00	45.63	L	C
ATOM	303	O	ALA	L	34	45.350	13.583	79.309	1.00	46.43	L	O
ATOM	304	CB	ALA	L	34	48.034	12.155	80.643	1.00	45.30	L	C
ATOM	305	N	CGU	L	35	45.225	11.360	79.637	1.00	45.00	L	N
ATOM	306	CA	CGU	L	35	44.274	11.132	78.559	1.00	44.45	L	C
ATOM	307	CB	CGU	L	35	43.892	9.646	78.502	1.00	47.50	L	C
ATOM	308	CG	CGU	L	35	45.001	8.586	78.399	1.00	52.62	L	C
ATOM	309	CD1	CGU	L	35	46.080	9.012	77.405	1.00	54.39	L	C
ATOM	310	CD2	CGU	L	35	45.632	8.287	79.763	1.00	53.62	L	C
ATOM	311	OE1	CGU	L	35	47.263	8.886	77.743	1.00	55.86	L	O
ATOM	312	OE2	CGU	L	35	45.722	9.460	76.313	1.00	56.24	L	O
ATOM	313	OE3	CGU	L	35	46.606	8.955	80.122	1.00	53.37	L	O
ATOM	314	OE4	CGU	L	35	45.140	7.379	80.445	1.00	54.53	L	O
ATOM	315	C	CGU	L	35	43.019	11.992	78.756	1.00	42.91	L	C
ATOM	316	O	CGU	L	35	42.540	12.632	77.819	1.00	42.37	L	O
ATOM	317	N	ARG	L	36	42.494	12.009	79.978	1.00	40.60	L	N
ATOM	318	CA	ARG	L	36	41.304	12.795	80.294	1.00	38.99	L	C
ATOM	319	C	ARG	L	36	41.572	14.296	80.212	1.00	36.95	L	C
ATOM	320	O	ARG	L	36	40.728	15.061	79.747	1.00	36.47	L	O
ATOM	321	CB	ARG	L	36	40.797	12.447	81.696	1.00	41.08	L	C
ATOM	322	CG	ARG	L	36	40.298	11.017	81.844	1.00	43.46	L	C
ATOM	323	CD	ARG	L	36	39.891	10.718	83.278	1.00	45.24	L	C
ATOM	324	NE	ARG	L	36	39.441	9.337	83.441	1.00	47.54	L	N
ATOM	325	CZ	ARG	L	36	39.133	8.776	84.607	1.00	48.41	L	C
ATOM	326	NH1	ARG	L	36	39.225	9.471	85.734	1.00	46.77	L	N
ATOM	327	NH2	ARG	L	36	38.728	7.512	84.647	1.00	50.53	L	N

ATOM	328	N	THR	L	37	42.747	14.716	80.669	1.00	34.62	L	N
ATOM	329	CA	THR	L	37	43.109	16.126	80.640	1.00	32.74	L	C
ATOM	330	C	THR	L	37	43.201	16.637	79.204	1.00	31.75	L	C
ATOM	331	O	THR	L	37	42.694	17.714	78.891	1.00	30.68	L	O
ATOM	332	CB	THR	L	37	44.455	16.369	81.351	1.00	32.46	L	C
ATOM	333	OG1	THR	L	37	44.393	15.839	82.681	1.00	32.01	L	O
ATOM	334	CG2	THR	L	37	44.759	17.861	81.427	1.00	31.14	L	C
ATOM	335	N	LYS	L	38	43.844	15.860	78.336	1.00	31.24	L	N
ATOM	336	CA	LYS	L	38	43.989	16.239	76.934	1.00	32.20	L	C
ATOM	337	C	LYS	L	38	42.630	16.318	76.233	1.00	30.65	L	C
ATOM	338	O	LYS	L	38	42.390	17.231	75.446	1.00	31.32	L	O
ATOM	339	CB	LYS	L	38	44.891	15.241	76.197	1.00	34.59	L	C
ATOM	340	CG	LYS	L	38	46.332	15.182	76.711	1.00	37.74	L	C
ATOM	341	CD	LYS	L	38	47.030	16.539	76.640	1.00	39.00	L	C
ATOM	342	CE	LYS	L	38	47.216	17.009	75.204	1.00	41.05	L	C
ATOM	343	NZ	LYS	L	38	47.824	18.365	75.130	1.00	38.92	L	N
ATOM	344	N	LEU	L	39	41.749	15.362	76.519	1.00	28.80	L	N
ATOM	345	CA	LEU	L	39	40.417	15.345	75.919	1.00	28.45	L	C
ATOM	346	C	LEU	L	39	39.665	16.624	76.275	1.00	27.55	L	C
ATOM	347	O	LEU	L	39	38.927	17.170	75.458	1.00	27.44	L	O
ATOM	348	CB	LEU	L	39	39.619	14.134	76.410	1.00	28.33	L	C
ATOM	349	CG	LEU	L	39	38.190	14.034	75.866	1.00	30.67	L	C
ATOM	350	CD1	LEU	L	39	38.228	13.988	74.342	1.00	30.91	L	C
ATOM	351	CD2	LEU	L	39	37.504	12.791	76.422	1.00	30.33	L	C
ATOM	352	N	PHE	L	40	39.850	17.091	77.505	1.00	26.66	L	N
ATOM	353	CA	PHE	L	40	39.213	18.315	77.968	1.00	26.79	L	C
ATOM	354	C	PHE	L	40	39.869	19.531	77.319	1.00	26.64	L	C
ATOM	355	O	PHE	L	40	39.188	20.429	76.821	1.00	27.35	L	O
ATOM	356	CB	PHE	L	40	39.346	18.438	79.491	1.00	25.08	L	C
ATOM	357	CG	PHE	L	40	39.028	19.810	80.020	1.00	25.21	L	C
ATOM	358	CD1	PHE	L	40	37.707	20.208	80.225	1.00	24.16	L	C
ATOM	359	CD2	PHE	L	40	40.052	20.718	80.291	1.00	24.18	L	C
ATOM	360	CE1	PHE	L	40	37.411	21.488	80.692	1.00	25.10	L	C
ATOM	361	CE2	PHE	L	40	39.767	22.003	80.758	1.00	24.75	L	C
ATOM	362	CZ	PHE	L	40	38.444	22.389	80.959	1.00	25.22	L	C
ATOM	363	N	TRP	L	41	41.199	19.539	77.324	1.00	25.96	L	N
ATOM	364	CA	TRP	L	41	41.990	20.648	76.795	1.00	26.28	L	C
ATOM	365	C	TRP	L	41	41.866	20.970	75.301	1.00	27.29	L	C
ATOM	366	O	TRP	L	41	41.988	22.131	74.906	1.00	26.04	L	O
ATOM	367	CB	TRP	L	41	43.464	20.425	77.144	1.00	24.26	L	C
ATOM	368	CG	TRP	L	41	44.306	21.652	77.027	1.00	25.36	L	C
ATOM	369	CD1	TRP	L	41	45.257	21.906	76.086	1.00	25.02	L	C
ATOM	370	CD2	TRP	L	41	44.270	22.802	77.883	1.00	25.54	L	C
ATOM	371	NE1	TRP	L	41	45.819	23.143	76.299	1.00	27.28	L	N
ATOM	372	CE2	TRP	L	41	45.232	23.715	77.395	1.00	26.01	L	C
ATOM	373	CE3	TRP	L	41	43.517	23.149	79.014	1.00	26.85	L	C
ATOM	374	CZ2	TRP	L	41	45.464	24.954	78.000	1.00	24.01	L	C
ATOM	375	CZ3	TRP	L	41	43.747	24.383	79.616	1.00	25.86	L	C
ATOM	376	CH2	TRP	L	41	44.715	25.270	79.105	1.00	26.46	L	C
ATOM	377	N	ILE	L	42	41.629	19.968	74.463	1.00	28.66	L	N
ATOM	378	CA	ILE	L	42	41.523	20.237	73.033	1.00	30.71	L	C
ATOM	379	C	ILE	L	42	40.370	21.171	72.666	1.00	29.53	L	C
ATOM	380	O	ILE	L	42	40.469	21.936	71.705	1.00	30.98	L	O
ATOM	381	CB	ILE	L	42	41.429	18.925	72.209	1.00	32.87	L	C
ATOM	382	CG1	ILE	L	42	40.350	18.004	72.771	1.00	33.91	L	C
ATOM	383	CG2	ILE	L	42	42.769	18.217	72.217	1.00	36.59	L	C

ATOM	384	CD1	ILE	L	42	38.982	18.321	72.269	1.00	36.99	L	C
ATOM	385	N	SER	L	43	39.289	21.127	73.437	1.00	28.62	L	N
ATOM	386	CA	SER	L	43	38.136	21.985	73.185	1.00	28.31	L	C
ATOM	387	C	SER	L	43	38.213	23.262	74.009	1.00	27.84	L	C
ATOM	388	O	SER	L	43	37.980	24.356	73.499	1.00	27.48	L	O
ATOM	389	CB	SER	L	43	36.839	21.247	73.517	1.00	26.23	L	C
ATOM	390	OG	SER	L	43	36.679	20.123	72.671	1.00	27.51	L	O
ATOM	391	N	TYR	L	44	38.541	23.115	75.289	1.00	27.54	L	N
ATOM	392	CA	TYR	L	44	38.640	24.257	76.188	1.00	27.08	L	C
ATOM	393	C	TYR	L	44	39.581	25.329	75.650	1.00	27.23	L	C
ATOM	394	O	TYR	L	44	39.241	26.510	75.650	1.00	27.59	L	O
ATOM	395	CB	TYR	L	44	39.136	23.805	77.567	1.00	26.19	L	C
ATOM	396	CG	TYR	L	44	39.140	24.898	78.614	1.00	24.94	L	C
ATOM	397	CD1	TYR	L	44	37.949	25.366	79.164	1.00	23.63	L	C
ATOM	398	CD2	TYR	L	44	40.337	25.457	79.064	1.00	26.53	L	C
ATOM	399	CE1	TYR	L	44	37.949	26.362	80.142	1.00	26.54	L	C
ATOM	400	CE2	TYR	L	44	40.348	26.455	80.043	1.00	26.05	L	C
ATOM	401	CZ	TYR	L	44	39.151	26.899	80.577	1.00	26.97	L	C
ATOM	402	OH	TYR	L	44	39.150	27.865	81.560	1.00	28.80	L	O
ATOM	403	N	SER	L	45	40.757	24.911	75.192	1.00	27.72	L	N
ATOM	404	CA	SER	L	45	41.768	25.839	74.686	1.00	30.15	L	C
ATOM	405	C	SER	L	45	41.744	26.104	73.182	1.00	30.62	L	C
ATOM	406	O	SER	L	45	42.604	26.820	72.671	1.00	30.63	L	O
ATOM	407	CB	SER	L	45	43.165	25.340	75.061	1.00	30.16	L	C
ATOM	408	OG	SER	L	45	43.497	24.166	74.339	1.00	29.88	L	O
ATOM	409	N	ASP	L	46	40.771	25.543	72.472	1.00	31.14	L	N
ATOM	410	CA	ASP	L	46	40.703	25.745	71.027	1.00	31.20	L	C
ATOM	411	C	ASP	L	46	40.411	27.189	70.627	1.00	30.32	L	C
ATOM	412	O	ASP	L	46	40.884	27.650	69.594	1.00	32.57	L	O
ATOM	413	CB	ASP	L	46	39.646	24.833	70.405	1.00	31.05	L	C
ATOM	414	CG	ASP	L	46	39.742	24.784	68.892	1.00	32.56	L	C
ATOM	415	OD1	ASP	L	46	40.634	24.106	68.375	1.00	33.28	L	O
ATOM	416	OD2	ASP	L	46	38.941	25.428	68.242	1.00	29.30	L	O
ATOM	417	N	GLY	L	47	39.636	27.899	71.442	1.00	29.23	L	N
ATOM	418	CA	GLY	L	47	39.299	29.276	71.131	1.00	28.60	L	C
ATOM	419	C	GLY	L	47	38.100	29.318	70.202	1.00	31.30	L	C
ATOM	420	O	GLY	L	47	37.926	28.417	69.392	1.00	30.95	L	O
ATOM	421	N	ASP	L	48	37.273	30.355	70.308	1.00	31.54	L	N
ATOM	422	CA	ASP	L	48	36.090	30.472	69.462	1.00	32.74	L	C
ATOM	423	C	ASP	L	48	36.378	31.223	68.165	1.00	33.54	L	C
ATOM	424	O	ASP	L	48	36.498	32.452	68.159	1.00	32.67	L	O
ATOM	425	CB	ASP	L	48	34.970	31.168	70.240	1.00	34.96	L	C
ATOM	426	CG	ASP	L	48	33.809	31.573	69.358	1.00	36.81	L	C
ATOM	427	OD1	ASP	L	48	33.501	30.848	68.425	1.00	36.52	L	O
ATOM	428	OD2	ASP	L	48	33.208	32.615	69.623	1.00	39.87	L	O
ATOM	429	N	GLN	L	49	36.485	30.481	67.064	1.00	33.17	L	N
ATOM	430	CA	GLN	L	49	36.767	31.089	65.762	1.00	33.44	L	C
ATOM	431	C	GLN	L	49	35.666	32.022	65.259	1.00	33.32	L	C
ATOM	432	O	GLN	L	49	35.871	32.774	64.305	1.00	34.51	L	O
ATOM	433	CB	GLN	L	49	37.046	30.009	64.713	1.00	32.45	L	C
ATOM	434	CG	GLN	L	49	38.448	29.410	64.780	1.00	31.73	L	C
ATOM	435	CD	GLN	L	49	38.707	28.668	66.078	1.00	33.97	L	C
ATOM	436	OE1	GLN	L	49	37.915	27.822	66.477	1.00	32.13	L	O
ATOM	437	NE2	GLN	L	49	39.821	28.978	66.737	1.00	32.44	L	N
ATOM	438	N	CYS	L	50	34.500	31.973	65.895	1.00	32.75	L	N
ATOM	439	CA	CYS	L	50	33.391	32.840	65.519	1.00	32.95	L	C

ATOM	440	C	CYS	L	50	33.533	34.239	66.113	1.00	34.35	L	C
ATOM	441	O	CYS	L	50	32.803	35.154	65.733	1.00	33.23	L	O
ATOM	442	CB	CYS	L	50	32.062	32.249	65.988	1.00	31.79	L	C
ATOM	443	SG	CYS	L	50	31.419	30.890	64.967	1.00	30.41	L	S
ATOM	444	N	ALA	L	51	34.466	34.398	67.049	1.00	36.39	L	N
ATOM	445	CA	ALA	L	51	34.698	35.681	67.712	1.00	38.60	L	C
ATOM	446	C	ALA	L	51	34.967	36.818	66.727	1.00	39.03	L	C
ATOM	447	O	ALA	L	51	34.554	37.955	66.952	1.00	39.61	L	O
ATOM	448	CB	ALA	L	51	35.861	35.554	68.695	1.00	37.84	L	C
ATOM	449	N	GSERL		52	35.657	36.507	65.636	1.00	39.50	L	N
ATOM	450	CA	GSERL		52	35.974	37.503	64.619	1.00	39.27	L	C
ATOM	451	CB	GSERL		52	37.114	36.982	63.737	1.00	40.23	L	C
ATOM	452	OG	GSERL		52	36.756	36.974	62.365	1.00	45.10	L	O
ATOM	453	C	GSERL		52	34.756	37.859	63.760	1.00	38.60	L	C
ATOM	454	O	GSERL		52	34.854	38.667	62.835	1.00	38.29	L	O
ATOM	455	C1	GSERL		52	37.197	35.776	61.707	1.00	45.99	L	C
ATOM	456	C2	GSERL		52	38.111	36.101	60.515	1.00	46.11	L	C
ATOM	457	C3	GSERL		52	38.477	34.801	59.788	1.00	46.60	L	C
ATOM	458	C4	GSERL		52	39.100	33.808	60.777	1.00	46.16	L	C
ATOM	459	C5	GSERL		52	38.180	33.615	62.004	1.00	46.88	L	C
ATOM	460	C6	GSERL		52	38.849	32.688	63.024	1.00	48.42	L	C
ATOM	461	O2	GSERL		52	37.438	36.988	59.614	1.00	47.32	L	O
ATOM	462	O3	GSERL		52	39.406	35.079	58.734	1.00	46.42	L	O
ATOM	463	O4	GSERL		52	39.302	32.549	60.123	1.00	46.46	L	O
ATOM	464	O5	GSERL		52	37.851	34.874	62.616	1.00	47.23	L	O
ATOM	465	O6	GSERL		52	39.251	31.462	62.431	1.00	51.52	L	O
ATOM	466	N	SER	L	53	33.610	37.263	64.085	1.00	36.60	L	N
ATOM	467	CA	SER	L	53	32.367	37.488	63.354	1.00	35.81	L	C
ATOM	468	C	SER	L	53	32.602	37.463	61.845	1.00	33.73	L	C
ATOM	469	O	SER	L	53	32.395	38.460	61.162	1.00	33.37	L	O
ATOM	470	CB	SER	L	53	31.765	38.831	63.764	1.00	37.62	L	C
ATOM	471	OG	SER	L	53	32.684	39.879	63.524	1.00	40.28	L	O
ATOM	472	N	PRO	L	54	33.026	36.310	61.303	1.00	32.42	L	N
ATOM	473	CA	PRO	L	54	33.285	36.192	59.865	1.00	31.65	L	C
ATOM	474	C	PRO	L	54	32.069	36.078	58.940	1.00	30.67	L	C
ATOM	475	O	PRO	L	54	32.156	36.424	57.761	1.00	30.19	L	O
ATOM	476	CB	PRO	L	54	34.172	34.956	59.788	1.00	31.82	L	C
ATOM	477	CG	PRO	L	54	33.578	34.084	60.841	1.00	30.71	L	C
ATOM	478	CD	PRO	L	54	33.366	35.051	61.994	1.00	30.98	L	C
ATOM	479	N	CYS	L	55	30.946	35.594	59.461	1.00	29.86	L	N
ATOM	480	CA	CYS	L	55	29.752	35.422	58.635	1.00	30.36	L	C
ATOM	481	C	CYS	L	55	29.033	36.733	58.343	1.00	31.54	L	C
ATOM	482	O	CYS	L	55	28.455	37.358	59.230	1.00	32.38	L	O
ATOM	483	CB	CYS	L	55	28.794	34.430	59.290	1.00	28.02	L	C
ATOM	484	SG	CYS	L	55	29.586	32.875	59.818	1.00	28.74	L	S
ATOM	485	N	GLN	L	56	29.060	37.122	57.074	1.00	31.32	L	N
ATOM	486	CA	GLN	L	56	28.456	38.365	56.607	1.00	30.45	L	C
ATOM	487	C	GLN	L	56	26.983	38.271	56.217	1.00	29.58	L	C
ATOM	488	O	GLN	L	56	26.387	37.195	56.205	1.00	30.14	L	O
ATOM	489	CB	GLN	L	56	29.239	38.873	55.398	1.00	29.51	L	C
ATOM	490	CG	GLN	L	56	30.731	38.996	55.615	1.00	27.82	L	C
ATOM	491	CD	GLN	L	56	31.463	39.252	54.321	1.00	28.65	L	C
ATOM	492	OE1	GLN	L	56	31.054	40.098	53.526	1.00	31.65	L	O
ATOM	493	NE2	GLN	L	56	32.551	38.526	54.098	1.00	29.31	L	N
ATOM	494	N	ASN	L	57	26.415	39.429	55.897	1.00	30.03	L	N
ATOM	495	CA	ASN	L	57	25.030	39.559	55.453	1.00	29.58	L	C

ATOM	496	C	ASN	L	57	23.952	38.887	56.296	1.00	29.62	L	C
ATOM	497	O	ASN	L	57	23.024	38.276	55.764	1.00	29.77	L	O
ATOM	498	CB	ASN	L	57	24.921	39.085	53.999	1.00	29.04	L	C
ATOM	499	CG	ASN	L	57	25.762	39.924	53.054	1.00	29.56	L	C
ATOM	500	OD1	ASN	L	57	25.568	41.134	52.945	1.00	32.62	L	O
ATOM	501	ND2	ASN	L	57	26.702	39.287	52.367	1.00	29.28	L	N
ATOM	502	N	GLY	L	58	24.059	39.019	57.610	1.00	30.01	L	N
ATOM	503	CA	GLY	L	58	23.061	38.432	58.485	1.00	30.78	L	C
ATOM	504	C	GLY	L	58	23.145	36.931	58.670	1.00	30.82	L	C
ATOM	505	O	GLY	L	58	22.166	36.299	59.066	1.00	31.08	L	O
ATOM	506	N	GLY	L	59	24.305	36.351	58.388	1.00	31.24	L	N
ATOM	507	CA	GLY	L	59	24.453	34.919	58.557	1.00	31.81	L	C
ATOM	508	C	GLY	L	59	24.692	34.578	60.015	1.00	31.05	L	C
ATOM	509	O	GLY	L	59	24.845	35.466	60.853	1.00	31.54	L	O
ATOM	510	N	FSERL		60	24.723	33.289	60.326	1.00	30.80	L	N
ATOM	511	CA	FSERL		60	24.959	32.852	61.690	1.00	30.86	L	C
ATOM	512	CB	FSERL		60	23.724	32.128	62.227	1.00	31.58	L	C
ATOM	513	OG	FSERL		60	22.643	33.041	62.308	1.00	32.58	L	O
ATOM	514	C	FSERL		60	26.184	31.953	61.743	1.00	30.82	L	C
ATOM	515	O	FSERL		60	26.297	30.990	60.984	1.00	29.56	L	O
ATOM	516	C1	FSERL		60	21.375	32.378	62.268	1.00	35.22	L	C
ATOM	517	C2	FSERL		60	20.246	33.387	62.560	1.00	36.79	L	C
ATOM	518	C3	FSERL		60	20.174	34.428	61.430	1.00	37.43	L	C
ATOM	519	C4	FSERL		60	20.031	33.715	60.084	1.00	36.10	L	C
ATOM	520	C5	FSERL		60	21.164	32.683	59.913	1.00	35.80	L	C
ATOM	521	C6	FSERL		60	21.036	31.969	58.566	1.00	35.30	L	C
ATOM	522	O2	FSERL		60	20.509	34.051	63.802	1.00	39.97	L	O
ATOM	523	O3	FSERL		60	19.049	35.291	61.638	1.00	39.35	L	O
ATOM	524	O4	FSERL		60	18.764	33.048	60.034	1.00	38.01	L	O
ATOM	525	O5	FSERL		60	21.172	31.739	60.996	1.00	35.11	L	O
ATOM	526	N	CYS	L	61	27.103	32.284	62.644	1.00	29.76	L	N
ATOM	527	CA	CYS	L	61	28.340	31.532	62.803	1.00	30.26	L	C
ATOM	528	C	CYS	L	61	28.205	30.412	63.825	1.00	30.72	L	C
ATOM	529	O	CYS	L	61	27.616	30.591	64.895	1.00	29.55	L	O
ATOM	530	CB	CYS	L	61	29.468	32.474	63.227	1.00	29.48	L	C
ATOM	531	SG	CYS	L	61	31.145	31.764	63.150	1.00	30.89	L	S
ATOM	532	N	LYS	L	62	28.754	29.254	63.477	1.00	30.27	L	N
ATOM	533	CA	LYS	L	62	28.729	28.090	64.347	1.00	29.64	L	C
ATOM	534	C	LYS	L	62	30.183	27.688	64.543	1.00	29.26	L	C
ATOM	535	O	LYS	L	62	30.870	27.312	63.595	1.00	28.28	L	O
ATOM	536	CB	LYS	L	62	27.943	26.952	63.696	1.00	30.78	L	C
ATOM	537	CG	LYS	L	62	27.561	25.826	64.642	1.00	33.70	L	C
ATOM	538	CD	LYS	L	62	28.780	25.112	65.204	1.00	35.68	L	C
ATOM	539	CE	LYS	L	62	28.392	23.957	66.122	1.00	34.05	L	C
ATOM	540	NZ	LYS	L	62	27.581	24.389	67.286	1.00	32.19	L	N
ATOM	541	N	ASP	L	63	30.645	27.781	65.782	1.00	29.03	L	N
ATOM	542	CA	ASP	L	63	32.018	27.455	66.120	1.00	28.45	L	C
ATOM	543	C	ASP	L	63	32.317	25.970	65.961	1.00	27.88	L	C
ATOM	544	O	ASP	L	63	31.489	25.120	66.286	1.00	26.64	L	O
ATOM	545	CB	ASP	L	63	32.310	27.909	67.546	1.00	28.61	L	C
ATOM	546	CG	ASP	L	63	33.762	27.778	67.899	1.00	31.76	L	C
ATOM	547	OD1	ASP	L	63	34.595	28.171	67.072	1.00	29.78	L	O
ATOM	548	OD2	ASP	L	63	34.057	27.289	68.989	1.00	31.88	L	O
ATOM	549	N	GLN	L	64	33.511	25.670	65.463	1.00	27.71	L	N
ATOM	550	CA	GLN	L	64	33.934	24.296	65.222	1.00	29.46	L	C
ATOM	551	C	GLN	L	64	35.354	24.115	65.751	1.00	29.86	L	C

ATOM	552	O	GLN	L	64	35.988	25.076	66.145	1.00	29.22	L	O
ATOM	553	CB	GLN	L	64	33.894	24.014	63.715	1.00	30.77	L	C
ATOM	554	CG	GLN	L	64	33.597	22.576	63.346	1.00	33.56	L	C
ATOM	555	CD	GLN	L	64	32.157	22.156	63.621	1.00	33.54	L	C
ATOM	556	OE1	GLN	L	64	31.840	20.973	63.568	1.00	36.28	L	O
ATOM	557	NE2	GLN	L	64	31.284	23.119	63.904	1.00	31.18	L	N
ATOM	558	N	LEU	L	65	35.862	22.891	65.740	1.00	32.40	L	N
ATOM	559	CA	LEU	L	65	37.206	22.633	66.242	1.00	33.87	L	C
ATOM	560	C	LEU	L	65	38.292	23.203	65.332	1.00	35.15	L	C
ATOM	561	O	LEU	L	65	38.688	22.574	64.349	1.00	36.47	L	O
ATOM	562	CB	LEU	L	65	37.410	21.125	66.422	1.00	35.23	L	C
ATOM	563	CG	LEU	L	65	38.554	20.679	67.337	1.00	36.14	L	C
ATOM	564	CD1	LEU	L	65	38.435	21.372	68.687	1.00	36.95	L	C
ATOM	565	CD2	LEU	L	65	38.503	19.172	67.517	1.00	35.86	L	C
ATOM	566	N	GLN	L	66	38.767	24.401	65.666	1.00	35.72	L	N
ATOM	567	CA	GLN	L	66	39.820	25.072	64.903	1.00	35.89	L	C
ATOM	568	C	GLN	L	66	39.293	25.586	63.561	1.00	35.00	L	C
ATOM	569	O	GLN	L	66	39.998	25.562	62.547	1.00	33.68	L	O
ATOM	570	CB	GLN	L	66	40.986	24.101	64.674	1.00	37.22	L	C
ATOM	571	CG	GLN	L	66	42.288	24.748	64.232	1.00	40.93	L	C
ATOM	572	CD	GLN	L	66	43.040	25.456	65.356	1.00	40.68	L	C
ATOM	573	OE1	GLN	L	66	44.109	26.017	65.128	1.00	41.86	L	O
ATOM	574	NE2	GLN	L	66	42.488	25.431	66.566	1.00	40.50	L	N
ATOM	575	N	SER	L	67	38.051	26.059	63.568	1.00	31.83	L	N
ATOM	576	CA	SER	L	67	37.412	26.568	62.365	1.00	31.03	L	C
ATOM	577	C	SER	L	67	35.991	27.036	62.667	1.00	31.16	L	C
ATOM	578	O	SER	L	67	35.613	27.197	63.829	1.00	31.27	L	O
ATOM	579	CB	SER	L	67	37.389	25.477	61.288	1.00	30.23	L	C
ATOM	580	OG	SER	L	67	36.946	24.239	61.817	1.00	30.96	L	O
ATOM	581	N	TYR	L	68	35.210	27.265	61.618	1.00	29.96	L	N
ATOM	582	CA	TYR	L	68	33.835	27.707	61.785	1.00	28.95	L	C
ATOM	583	C	TYR	L	68	32.987	27.358	60.573	1.00	28.08	L	C
ATOM	584	O	TYR	L	68	33.500	26.977	59.516	1.00	27.87	L	O
ATOM	585	CB	TYR	L	68	33.769	29.221	62.024	1.00	30.00	L	C
ATOM	586	CG	TYR	L	68	34.288	30.061	60.876	1.00	29.99	L	C
ATOM	587	CD1	TYR	L	68	35.650	30.332	60.743	1.00	30.22	L	C
ATOM	588	CD2	TYR	L	68	33.417	30.574	59.912	1.00	30.26	L	C
ATOM	589	CE1	TYR	L	68	36.135	31.090	59.682	1.00	29.23	L	C
ATOM	590	CE2	TYR	L	68	33.892	31.331	58.844	1.00	29.58	L	C
ATOM	591	CZ	TYR	L	68	35.251	31.585	58.737	1.00	29.30	L	C
ATOM	592	OH	TYR	L	68	35.733	32.320	57.683	1.00	28.26	L	O
ATOM	593	N	ILE	L	69	31.680	27.499	60.743	1.00	25.46	L	N
ATOM	594	CA	ILE	L	69	30.720	27.220	59.691	1.00	24.21	L	C
ATOM	595	C	ILE	L	69	29.732	28.374	59.657	1.00	23.58	L	C
ATOM	596	O	ILE	L	69	29.233	28.800	60.698	1.00	21.31	L	O
ATOM	597	CB	ILE	L	69	29.947	25.908	59.974	1.00	24.42	L	C
ATOM	598	CG1	ILE	L	69	30.904	24.717	59.914	1.00	24.57	L	C
ATOM	599	CG2	ILE	L	69	28.818	25.739	58.976	1.00	23.61	L	C
ATOM	600	CD1	ILE	L	69	30.243	23.389	60.201	1.00	23.77	L	C
ATOM	601	N	CYS	L	70	29.466	28.893	58.464	1.00	23.37	L	N
ATOM	602	CA	CYS	L	70	28.517	29.985	58.323	1.00	23.29	L	C
ATOM	603	C	CYS	L	70	27.195	29.499	57.730	1.00	24.32	L	C
ATOM	604	O	CYS	L	70	27.174	28.777	56.735	1.00	22.69	L	O
ATOM	605	CB	CYS	L	70	29.084	31.091	57.427	1.00	24.87	L	C
ATOM	606	SG	CYS	L	70	30.424	32.100	58.136	1.00	24.79	L	S
ATOM	607	N	PHE	L	71	26.096	29.880	58.373	1.00	23.47	L	N

ATOM	608	CA	PHE	L	71	24.765	29.550	57.896	1.00	24.42	L	C
ATOM	609	C	PHE	L	71	24.305	30.861	57.285	1.00	25.98	L	C
ATOM	610	O	PHE	L	71	24.271	31.884	57.961	1.00	26.06	L	O
ATOM	611	CB	PHE	L	71	23.840	29.148	59.051	1.00	23.72	L	C
ATOM	612	CG	PHE	L	71	24.079	27.753	59.563	1.00	23.26	L	C
ATOM	613	CD1	PHE	L	71	25.220	27.448	60.300	1.00	20.48	L	C
ATOM	614	CD2	PHE	L	71	23.170	26.737	59.286	1.00	21.74	L	C
ATOM	615	CE1	PHE	L	71	25.453	26.157	60.751	1.00	19.84	L	C
ATOM	616	CE2	PHE	L	71	23.395	25.440	59.733	1.00	22.58	L	C
ATOM	617	CZ	PHE	L	71	24.537	25.149	60.467	1.00	21.41	L	C
ATOM	618	N	CYS	L	72	23.964	30.838	56.004	1.00	27.38	L	N
ATOM	619	CA	CYS	L	72	23.561	32.060	55.322	1.00	28.04	L	C
ATOM	620	C	CYS	L	72	22.067	32.210	55.147	1.00	29.09	L	C
ATOM	621	O	CYS	L	72	21.315	31.236	55.240	1.00	30.40	L	O
ATOM	622	CB	CYS	L	72	24.216	32.125	53.941	1.00	27.64	L	C
ATOM	623	SG	CYS	L	72	25.997	31.758	53.929	1.00	27.84	L	S
ATOM	624	N	LEU	L	73	21.645	33.446	54.896	1.00	29.28	L	N
ATOM	625	CA	LEU	L	73	20.243	33.736	54.640	1.00	29.11	L	C
ATOM	626	C	LEU	L	73	20.018	33.294	53.201	1.00	29.05	L	C
ATOM	627	O	LEU	L	73	20.964	33.228	52.419	1.00	29.21	L	O
ATOM	628	CB	LEU	L	73	19.963	35.233	54.786	1.00	29.61	L	C
ATOM	629	CG	LEU	L	73	19.999	35.764	56.221	1.00	31.06	L	C
ATOM	630	CD1	LEU	L	73	19.802	37.274	56.220	1.00	32.08	L	C
ATOM	631	CD2	LEU	L	73	18.913	35.075	57.043	1.00	30.65	L	C
ATOM	632	N	PRO	L	74	18.766	32.991	52.833	1.00	29.36	L	N
ATOM	633	CA	PRO	L	74	18.384	32.543	51.492	1.00	29.38	L	C
ATOM	634	C	PRO	L	74	19.120	33.149	50.298	1.00	29.43	L	C
ATOM	635	O	PRO	L	74	19.630	32.420	49.449	1.00	29.02	L	O
ATOM	636	CB	PRO	L	74	16.888	32.828	51.461	1.00	30.46	L	C
ATOM	637	CG	PRO	L	74	16.486	32.477	52.854	1.00	29.08	L	C
ATOM	638	CD	PRO	L	74	17.570	33.151	53.682	1.00	29.95	L	C
ATOM	639	N	ALA	L	75	19.190	34.473	50.229	1.00	28.84	L	N
ATOM	640	CA	ALA	L	75	19.849	35.124	49.100	1.00	28.32	L	C
ATOM	641	C	ALA	L	75	21.368	35.226	49.194	1.00	27.93	L	C
ATOM	642	O	ALA	L	75	21.978	36.020	48.481	1.00	29.61	L	O
ATOM	643	CB	ALA	L	75	19.257	36.508	48.893	1.00	27.56	L	C
ATOM	644	N	PHE	L	76	21.987	34.418	50.047	1.00	26.68	L	N
ATOM	645	CA	PHE	L	76	23.433	34.480	50.205	1.00	25.92	L	C
ATOM	646	C	PHE	L	76	24.105	33.108	50.253	1.00	25.21	L	C
ATOM	647	O	PHE	L	76	23.484	32.103	50.606	1.00	24.64	L	O
ATOM	648	CB	PHE	L	76	23.770	35.269	51.479	1.00	26.98	L	C
ATOM	649	CG	PHE	L	76	23.308	36.705	51.447	1.00	26.03	L	C
ATOM	650	CD1	PHE	L	76	24.009	37.660	50.717	1.00	26.24	L	C
ATOM	651	CD2	PHE	L	76	22.161	37.094	52.128	1.00	25.56	L	C
ATOM	652	CE1	PHE	L	76	23.570	38.986	50.665	1.00	27.46	L	C
ATOM	653	CE2	PHE	L	76	21.713	38.416	52.083	1.00	28.29	L	C
ATOM	654	CZ	PHE	L	76	22.420	39.363	51.350	1.00	27.25	L	C
ATOM	655	N	GLU	L	77	25.381	33.082	49.881	1.00	23.35	L	N
ATOM	656	CA	GLU	L	77	26.171	31.861	49.896	1.00	25.22	L	C
ATOM	657	C	GLU	L	77	27.636	32.260	50.022	1.00	25.48	L	C
ATOM	658	O	GLU	L	77	27.947	33.446	50.102	1.00	24.93	L	O
ATOM	659	CB	GLU	L	77	25.931	31.027	48.624	1.00	24.76	L	C
ATOM	660	CG	GLU	L	77	26.369	31.665	47.317	1.00	26.43	L	C
ATOM	661	CD	GLU	L	77	25.929	30.854	46.102	1.00	29.36	L	C
ATOM	662	OE1	GLU	L	77	26.332	29.708	45.975	1.00	26.59	L	O
ATOM	663	OE2	GLU	L	77	25.177	31.379	45.287	1.00	31.26	L	O

ATOM	664	N	GLY	L	78	28.525	31.273	50.045	1.00	24.82	L	N
ATOM	665	CA	GLY	L	78	29.944	31.545	50.191	1.00	24.72	L	C
ATOM	666	C	GLY	L	78	30.414	31.145	51.585	1.00	26.41	L	C
ATOM	667	O	GLY	L	78	29.613	31.056	52.513	1.00	25.52	L	O
ATOM	668	N	ARG	L	79	31.711	30.894	51.731	1.00	26.17	L	N
ATOM	669	CA	ARG	L	79	32.299	30.507	53.014	1.00	26.44	L	C
ATOM	670	C	ARG	L	79	31.847	31.428	54.146	1.00	27.39	L	C
ATOM	671	O	ARG	L	79	31.503	30.972	55.236	1.00	27.00	L	O
ATOM	672	CB	ARG	L	79	33.827	30.532	52.894	1.00	25.97	L	C
ATOM	673	CG	ARG	L	79	34.596	30.145	54.138	1.00	25.27	L	C
ATOM	674	CD	ARG	L	79	36.018	29.745	53.756	1.00	27.07	L	C
ATOM	675	NE	ARG	L	79	36.352	28.422	54.279	1.00	29.92	L	N
ATOM	676	CZ	ARG	L	79	37.168	27.553	53.689	1.00	31.71	L	C
ATOM	677	NH1	ARG	L	79	37.754	27.849	52.536	1.00	34.10	L	N
ATOM	678	NH2	ARG	L	79	37.394	26.375	54.254	1.00	34.56	L	N
ATOM	679	N	ASN	L	80	31.845	32.728	53.875	1.00	28.14	L	N
ATOM	680	CA	ASN	L	80	31.440	33.727	54.858	1.00	27.10	L	C
ATOM	681	C	ASN	L	80	30.171	34.446	54.415	1.00	27.35	L	C
ATOM	682	O	ASN	L	80	29.950	35.598	54.785	1.00	27.84	L	O
ATOM	683	CB	ASN	L	80	32.561	34.750	55.038	1.00	27.74	L	C
ATOM	684	CG	ASN	L	80	33.868	34.110	55.442	1.00	29.02	L	C
ATOM	685	OD1	ASN	L	80	33.952	33.449	56.473	1.00	31.37	L	O
ATOM	686	ND2	ASN	L	80	34.897	34.301	54.629	1.00	31.80	L	N
ATOM	687	N	CYS	L	81	29.348	33.771	53.616	1.00	26.38	L	N
ATOM	688	CA	CYS	L	81	28.103	34.353	53.113	1.00	26.94	L	C
ATOM	689	C	CYS	L	81	28.341	35.691	52.395	1.00	27.16	L	C
ATOM	690	O	CYS	L	81	27.474	36.566	52.392	1.00	26.50	L	O
ATOM	691	CB	CYS	L	81	27.115	34.563	54.263	1.00	26.45	L	C
ATOM	692	SG	CYS	L	81	26.764	33.080	55.267	1.00	28.68	L	S
ATOM	693	N	GLU	L	82	29.510	35.834	51.777	1.00	26.64	L	N
ATOM	694	CA	GLU	L	82	29.875	37.058	51.077	1.00	27.18	L	C
ATOM	695	C	GLU	L	82	29.314	37.153	49.654	1.00	27.98	L	C
ATOM	696	O	GLU	L	82	29.364	38.216	49.031	1.00	28.25	L	O
ATOM	697	CB	GLU	L	82	31.408	37.199	51.028	1.00	27.27	L	C
ATOM	698	CG	GLU	L	82	32.116	36.245	50.057	1.00	25.93	L	C
ATOM	699	CD	GLU	L	82	32.435	34.881	50.658	1.00	27.71	L	C
ATOM	700	OE1	GLU	L	82	31.618	34.339	51.391	1.00	26.78	L	O
ATOM	701	OE2	GLU	L	82	33.503	34.356	50.371	1.00	29.60	L	O
ATOM	702	N	THR	L	83	28.776	36.052	49.140	1.00	28.28	L	N
ATOM	703	CA	THR	L	83	28.238	36.042	47.784	1.00	28.62	L	C
ATOM	704	C	THR	L	83	26.762	36.405	47.698	1.00	29.44	L	C
ATOM	705	O	THR	L	83	25.910	35.738	48.284	1.00	28.89	L	O
ATOM	706	CB	THR	L	83	28.442	34.668	47.117	1.00	26.44	L	C
ATOM	707	OG1	THR	L	83	29.836	34.341	47.124	1.00	25.96	L	O
ATOM	708	CG2	THR	L	83	27.941	34.692	45.675	1.00	26.81	L	C
ATOM	709	N	HIS	L	84	26.475	37.472	46.958	1.00	31.51	L	N
ATOM	710	CA	HIS	L	84	25.109	37.939	46.759	1.00	34.54	L	C
ATOM	711	C	HIS	L	84	24.514	37.169	45.588	1.00	35.95	L	C
ATOM	712	O	HIS	L	84	24.914	37.372	44.442	1.00	36.09	L	O
ATOM	713	CB	HIS	L	84	25.085	39.434	46.424	1.00	36.24	L	C
ATOM	714	CG	HIS	L	84	25.439	40.328	47.572	1.00	38.81	L	C
ATOM	715	ND1	HIS	L	84	26.701	40.373	48.126	1.00	39.64	L	N
ATOM	716	CD2	HIS	L	84	24.697	41.231	48.256	1.00	39.06	L	C
ATOM	717	CE1	HIS	L	84	26.721	41.264	49.100	1.00	39.38	L	C
ATOM	718	NE2	HIS	L	84	25.518	41.799	49.200	1.00	41.56	L	N
ATOM	719	N	LYS	L	85	23.561	36.290	45.871	1.00	37.90	L	N

ATOM	720	CA	LYS	L	85	22.931	35.504	44.817	1.00	39.99	L	C
ATOM	721	C	LYS	L	85	22.179	36.379	43.808	1.00	41.95	L	C
ATOM	722	O	LYS	L	85	21.997	35.988	42.659	1.00	42.20	L	O
ATOM	723	CB	LYS	L	85	21.983	34.471	45.432	1.00	40.09	L	C
ATOM	724	CG	LYS	L	85	22.673	33.492	46.380	1.00	41.01	L	C
ATOM	725	CD	LYS	L	85	21.699	32.493	46.987	1.00	40.74	L	C
ATOM	726	CE	LYS	L	85	21.202	31.494	45.958	1.00	42.61	L	C
ATOM	727	NZ	LYS	L	85	22.296	30.609	45.462	1.00	43.27	L	N
ATOM	728	N	ASP	L	86	21.758	37.567	44.235	1.00	44.88	L	N
ATOM	729	CA	ASP	L	86	21.030	38.487	43.361	1.00	47.56	L	C
ATOM	730	C	ASP	L	86	21.941	39.324	42.455	1.00	47.92	L	C
ATOM	731	O	ASP	L	86	21.456	40.131	41.663	1.00	48.41	L	O
ATOM	732	CB	ASP	L	86	20.159	39.433	44.196	1.00	49.53	L	C
ATOM	733	CG	ASP	L	86	19.237	38.694	45.147	1.00	52.38	L	C
ATOM	734	OD1	ASP	L	86	18.537	37.783	44.701	1.00	53.34	L	O
ATOM	735	OD2	ASP	L	86	19.217	39.037	46.334	1.00	53.54	L	O
ATOM	736	N	ASP	L	87	23.252	39.132	42.568	1.00	48.29	L	N
ATOM	737	CA	ASP	L	87	24.213	39.883	41.762	1.00	48.43	L	C
ATOM	738	C	ASP	L	87	24.938	39.017	40.736	1.00	48.75	L	C
ATOM	739	O	ASP	L	87	26.108	39.250	40.431	1.00	48.28	L	O
ATOM	740	CB	ASP	L	87	25.244	40.550	42.673	1.00	49.27	L	C
ATOM	741	CG	ASP	L	87	24.639	41.629	43.545	1.00	49.65	L	C
ATOM	742	OD1	ASP	L	87	25.271	41.998	44.528	1.00	50.02	L	O
ATOM	743	OD2	ASP	L	87	23.541	42.101	43.231	1.00	50.10	L	O
ATOM	744	N	GLN	L	88	24.239	38.024	40.199	1.00	48.76	L	N
ATOM	745	CA	GLN	L	88	24.834	37.130	39.216	1.00	48.54	L	C
ATOM	746	C	GLN	L	88	24.028	37.101	37.921	1.00	47.25	L	C
ATOM	747	O	GLN	L	88	23.989	36.081	37.238	1.00	47.52	L	O
ATOM	748	CB	GLN	L	88	24.925	35.716	39.796	1.00	50.51	L	C
ATOM	749	CG	GLN	L	88	25.663	35.632	41.129	1.00	53.34	L	C
ATOM	750	CD	GLN	L	88	27.134	35.973	41.006	1.00	54.62	L	C
ATOM	751	OE1	GLN	L	88	27.499	37.016	40.461	1.00	55.79	L	O
ATOM	752	NE2	GLN	L	88	27.990	35.094	41.518	1.00	55.48	L	N
ATOM	753	N	LEU	L	89	23.399	38.221	37.575	1.00	45.19	L	N
ATOM	754	CA	LEU	L	89	22.587	38.294	36.363	1.00	42.20	L	C
ATOM	755	C	LEU	L	89	23.431	38.485	35.105	1.00	39.92	L	C
ATOM	756	O	LEU	L	89	23.313	39.493	34.407	1.00	39.00	L	O
ATOM	757	CB	LEU	L	89	21.564	39.429	36.487	1.00	42.79	L	C
ATOM	758	CG	LEU	L	89	20.458	39.493	35.430	1.00	43.04	L	C
ATOM	759	CD1	LEU	L	89	19.678	38.187	35.421	1.00	43.31	L	C
ATOM	760	CD2	LEU	L	89	19.532	40.662	35.729	1.00	43.24	L	C
ATOM	761	N	ILE	L	90	24.284	37.504	34.825	1.00	37.21	L	N
ATOM	762	CA	ILE	L	90	25.151	37.532	33.654	1.00	34.54	L	C
ATOM	763	C	ILE	L	90	24.832	36.325	32.778	1.00	33.42	L	C
ATOM	764	O	ILE	L	90	24.290	35.327	33.253	1.00	34.00	L	O
ATOM	765	CB	ILE	L	90	26.643	37.503	34.057	1.00	34.63	L	C
ATOM	766	CG1	ILE	L	90	26.934	36.263	34.905	1.00	33.21	L	C
ATOM	767	CG2	ILE	L	90	26.997	38.778	34.819	1.00	32.30	L	C
ATOM	768	CD1	ILE	L	90	28.372	36.154	35.356	1.00	36.32	L	C
ATOM	769	N	CYS	L	91	25.181	36.415	31.501	1.00	31.20	L	N
ATOM	770	CA	CYS	L	91	24.885	35.350	30.556	1.00	30.45	L	C
ATOM	771	C	CYS	L	91	25.471	33.971	30.833	1.00	30.35	L	C
ATOM	772	O	CYS	L	91	24.778	32.967	30.671	1.00	29.92	L	O
ATOM	773	CB	CYS	L	91	25.261	35.790	29.143	1.00	26.98	L	C
ATOM	774	SG	CYS	L	91	24.204	37.118	28.480	1.00	26.22	L	S
ATOM	775	N	VAL	L	92	26.732	33.902	31.245	1.00	29.06	L	N

ATOM	776	CA	VAL	L	92	27.333	32.602	31.514	1.00	28.75	L	C
ATOM	777	C	VAL	L	92	26.693	31.897	32.707	1.00	27.72	L	C
ATOM	778	O	VAL	L	92	26.940	30.712	32.937	1.00	28.52	L	O
ATOM	779	CB	VAL	L	92	28.866	32.709	31.718	1.00	31.07	L	C
ATOM	780	CG1	VAL	L	92	29.529	33.115	30.403	1.00	29.69	L	C
ATOM	781	CG2	VAL	L	92	29.190	33.717	32.813	1.00	31.06	L	C
ATOM	782	N	ASN	L	93	25.865	32.622	33.457	1.00	25.61	L	N
ATOM	783	CA	ASN	L	93	25.174	32.050	34.605	1.00	24.28	L	C
ATOM	784	C	ASN	L	93	23.753	31.651	34.213	1.00	23.30	L	C
ATOM	785	O	ASN	L	93	22.850	32.487	34.183	1.00	22.74	L	O
ATOM	786	CB	ASN	L	93	25.123	33.047	35.767	1.00	23.78	L	C
ATOM	787	CG	ASN	L	93	24.294	32.533	36.930	1.00	25.91	L	C
ATOM	788	OD1	ASN	L	93	24.175	31.326	37.128	1.00	28.42	L	O
ATOM	789	ND2	ASN	L	93	23.725	33.442	37.710	1.00	24.92	L	N
ATOM	790	N	GLU	L	94	23.564	30.370	33.907	1.00	22.36	L	N
ATOM	791	CA	GLU	L	94	22.257	29.862	33.511	1.00	22.33	L	C
ATOM	792	C	GLU	L	94	21.654	30.701	32.383	1.00	20.87	L	C
ATOM	793	O	GLU	L	94	20.472	31.047	32.412	1.00	18.77	L	O
ATOM	794	CB	GLU	L	94	21.302	29.856	34.711	1.00	24.83	L	C
ATOM	795	CG	GLU	L	94	21.714	28.934	35.863	1.00	27.12	L	C
ATOM	796	CD	GLU	L	94	21.684	27.462	35.488	1.00	30.61	L	C
ATOM	797	OE1	GLU	L	94	22.593	26.997	34.794	1.00	29.23	L	O
ATOM	798	OE2	GLU	L	94	20.741	26.783	35.891	1.00	35.59	L	O
ATOM	799	N	ASN	L	95	22.482	31.035	31.400	1.00	20.59	L	N
ATOM	800	CA	ASN	L	95	22.054	31.810	30.240	1.00	21.27	L	C
ATOM	801	C	ASN	L	95	21.375	33.134	30.603	1.00	22.32	L	C
ATOM	802	O	ASN	L	95	20.567	33.656	29.829	1.00	22.62	L	O
ATOM	803	CB	ASN	L	95	21.108	30.963	29.381	1.00	19.04	L	C
ATOM	804	CG	ASN	L	95	21.028	31.451	27.956	1.00	17.99	L	C
ATOM	805	OD1	ASN	L	95	22.040	31.546	27.270	1.00	20.44	L	O
ATOM	806	ND2	ASN	L	95	19.827	31.757	27.499	1.00	18.44	L	N
ATOM	807	N	GLY	L	96	21.716	33.674	31.773	1.00	23.58	L	N
ATOM	808	CA	GLY	L	96	21.140	34.928	32.227	1.00	22.26	L	C
ATOM	809	C	GLY	L	96	19.645	34.875	32.494	1.00	22.45	L	C
ATOM	810	O	GLY	L	96	19.002	35.911	32.650	1.00	24.38	L	O
ATOM	811	N	GLY	L	97	19.084	33.674	32.566	1.00	21.95	L	N
ATOM	812	CA	GLY	L	97	17.654	33.558	32.789	1.00	20.54	L	C
ATOM	813	C	GLY	L	97	16.871	33.760	31.501	1.00	20.22	L	C
ATOM	814	O	GLY	L	97	15.645	33.740	31.510	1.00	22.61	L	O
ATOM	815	N	CYS	L	98	17.580	33.959	30.393	1.00	19.38	L	N
ATOM	816	CA	CYS	L	98	16.956	34.161	29.086	1.00	20.02	L	C
ATOM	817	C	CYS	L	98	16.477	32.833	28.508	1.00	20.61	L	C
ATOM	818	O	CYS	L	98	17.165	31.818	28.623	1.00	20.27	L	O
ATOM	819	CB	CYS	L	98	17.955	34.764	28.105	1.00	19.41	L	C
ATOM	820	SG	CYS	L	98	18.601	36.419	28.485	1.00	22.10	L	S
ATOM	821	N	GLU	L	99	15.314	32.839	27.867	1.00	20.33	L	N
ATOM	822	CA	GLU	L	99	14.794	31.611	27.277	1.00	20.72	L	C
ATOM	823	C	GLU	L	99	15.625	31.164	26.076	1.00	19.15	L	C
ATOM	824	O	GLU	L	99	15.827	29.974	25.877	1.00	17.11	L	O
ATOM	825	CB	GLU	L	99	13.336	31.779	26.850	1.00	22.59	L	C
ATOM	826	CG	GLU	L	99	12.682	30.457	26.467	1.00	29.91	L	C
ATOM	827	CD	GLU	L	99	11.178	30.564	26.302	1.00	32.54	L	C
ATOM	828	OE1	GLU	L	99	10.738	31.204	25.370	1.00	33.67	L	O
ATOM	829	OE2	GLU	L	99	10.458	29.999	27.122	1.00	37.34	L	O
ATOM	830	N	GLN	L	100	16.101	32.114	25.274	1.00	18.04	L	N
ATOM	831	CA	GLN	L	100	16.911	31.763	24.112	1.00	18.31	L	C

ATOM	832	C	GLN	L	100	18.281	32.459	24.118	1.00	19.20	L C
ATOM	833	O	GLN	L	100	19.223	31.951	24.724	1.00	19.26	L O
ATOM	834	CB	GLN	L	100	16.145	32.056	22.805	1.00	16.04	L C
ATOM	835	CG	GLN	L	100	14.789	31.342	22.716	1.00	15.13	L C
ATOM	836	CD	GLN	L	100	14.182	31.366	21.321	1.00	16.10	L C
ATOM	837	OE1	GLN	L	100	14.478	32.245	20.520	1.00	16.54	L O
ATOM	838	NE2	GLN	L	100	13.314	30.403	21.034	1.00	17.14	L N
ATOM	839	N	TYR	L	101	18.408	33.610	23.465	1.00	19.40	L N
ATOM	840	CA	TYR	L	101	19.705	34.282	23.429	1.00	20.26	L C
ATOM	841	C	TYR	L	101	19.895	35.307	24.540	1.00	22.37	L C
ATOM	842	O	TYR	L	101	18.956	36.002	24.935	1.00	22.47	L O
ATOM	843	CB	TYR	L	101	19.934	34.955	22.071	1.00	18.52	L C
ATOM	844	CG	TYR	L	101	19.838	34.017	20.880	1.00	20.18	L C
ATOM	845	CD1	TYR	L	101	20.215	32.673	20.982	1.00	17.62	L C
ATOM	846	CD2	TYR	L	101	19.387	34.481	19.643	1.00	19.56	L C
ATOM	847	CE1	TYR	L	101	20.140	31.822	19.884	1.00	19.81	L C
ATOM	848	CE2	TYR	L	101	19.315	33.640	18.541	1.00	19.48	L C
ATOM	849	CZ	TYR	L	101	19.693	32.313	18.666	1.00	18.80	L C
ATOM	850	OH	TYR	L	101	19.641	31.489	17.564	1.00	19.13	L O
ATOM	851	N	CYS	L	102	21.127	35.387	25.032	1.00	22.05	L N
ATOM	852	CA	CYS	L	102	21.500	36.300	26.102	1.00	23.17	L C
ATOM	853	C	CYS	L	102	22.680	37.168	25.657	1.00	24.83	L C
ATOM	854	O	CYS	L	102	23.617	36.686	25.020	1.00	25.16	L O
ATOM	855	CB	CYS	L	102	21.897	35.494	27.343	1.00	22.80	L C
ATOM	856	SG	CYS	L	102	22.308	36.468	28.827	1.00	24.11	L S
ATOM	857	N	SER	L	103	22.628	38.451	25.995	1.00	26.62	L N
ATOM	858	CA	SER	L	103	23.695	39.382	25.650	1.00	28.86	L C
ATOM	859	C	SER	L	103	24.115	40.156	26.889	1.00	29.38	L C
ATOM	860	O	SER	L	103	23.277	40.759	27.558	1.00	31.61	L O
ATOM	861	CB	SER	L	103	23.225	40.377	24.584	1.00	27.37	L C
ATOM	862	OG	SER	L	103	22.975	39.733	23.350	1.00	29.37	L O
ATOM	863	N	ASP	L	104	25.405	40.125	27.205	1.00	30.25	L N
ATOM	864	CA	ASP	L	104	25.915	40.865	28.352	1.00	31.60	L C
ATOM	865	C	ASP	L	104	26.112	42.304	27.899	1.00	33.46	L C
ATOM	866	O	ASP	L	104	26.323	42.562	26.714	1.00	32.44	L O
ATOM	867	CB	ASP	L	104	27.258	40.303	28.820	1.00	30.24	L C
ATOM	868	CG	ASP	L	104	27.124	38.978	29.537	1.00	31.11	L C
ATOM	869	OD1	ASP	L	104	26.369	38.909	30.503	1.00	30.36	L O
ATOM	870	OD2	ASP	L	104	27.788	38.022	29.129	1.00	31.46	L O
ATOM	871	N	HIS	L	105	26.045	43.241	28.835	1.00	37.03	L N
ATOM	872	CA	HIS	L	105	26.226	44.642	28.486	1.00	40.26	L C
ATOM	873	C	HIS	L	105	27.048	45.418	29.505	1.00	43.18	L C
ATOM	874	O	HIS	L	105	26.942	45.197	30.714	1.00	42.14	L O
ATOM	875	CB	HIS	L	105	24.866	45.317	28.288	1.00	38.90	L C
ATOM	876	CG	HIS	L	105	24.151	44.878	27.048	1.00	38.94	L C
ATOM	877	ND1	HIS	L	105	24.678	45.051	25.786	1.00	38.12	L N
ATOM	878	CD2	HIS	L	105	22.955	44.267	26.875	1.00	37.83	L C
ATOM	879	CE1	HIS	L	105	23.838	44.565	24.890	1.00	38.48	L C
ATOM	880	NE2	HIS	L	105	22.785	44.083	25.524	1.00	37.45	L N
ATOM	881	N	THR	L	106	27.875	46.325	28.993	1.00	46.90	L N
ATOM	882	CA	THR	L	106	28.731	47.171	29.816	1.00	49.56	L C
ATOM	883	C	THR	L	106	27.995	48.481	30.076	1.00	49.91	L C
ATOM	884	O	THR	L	106	27.876	49.319	29.182	1.00	51.77	L O
ATOM	885	CB	THR	L	106	30.061	47.482	29.093	1.00	50.44	L C
ATOM	886	OG1	THR	L	106	30.719	46.256	28.752	1.00	52.50	L O
ATOM	887	CG2	THR	L	106	30.977	48.310	29.983	1.00	51.29	L C

ATOM	888	N	GLY	L	107	27.499	48.650	31.297	1.00	50.05	L	N
ATOM	889	CA	GLY	L	107	26.772	49.862	31.637	1.00	50.24	L	C
ATOM	890	C	GLY	L	107	25.265	49.664	31.683	1.00	50.91	L	C
ATOM	891	O	GLY	L	107	24.524	50.566	32.076	1.00	51.47	L	O
ATOM	892	N	THR	L	108	24.812	48.480	31.276	1.00	50.46	L	N
ATOM	893	CA	THR	L	108	23.394	48.138	31.269	1.00	48.90	L	C
ATOM	894	C	THR	L	108	23.244	46.633	31.482	1.00	47.11	L	C
ATOM	895	O	THR	L	108	24.024	45.847	30.948	1.00	47.64	L	O
ATOM	896	CB	THR	L	108	22.733	48.524	29.929	1.00	50.40	L	C
ATOM	897	OG1	THR	L	108	23.506	47.998	28.842	1.00	51.52	L	O
ATOM	898	CG2	THR	L	108	22.639	50.038	29.793	1.00	51.68	L	C
ATOM	899	N	LYS	L	109	22.244	46.238	32.266	1.00	44.24	L	N
ATOM	900	CA	LYS	L	109	22.005	44.825	32.558	1.00	41.00	L	C
ATOM	901	C	LYS	L	109	21.909	43.997	31.280	1.00	37.67	L	C
ATOM	902	O	LYS	L	109	21.642	44.531	30.201	1.00	37.06	L	O
ATOM	903	CB	LYS	L	109	20.716	44.663	33.367	1.00	42.02	L	C
ATOM	904	CG	LYS	L	109	19.450	44.860	32.555	1.00	44.84	L	C
ATOM	905	CD	LYS	L	109	18.219	44.906	33.444	1.00	47.58	L	C
ATOM	906	CE	LYS	L	109	18.148	46.209	34.230	1.00	49.04	L	C
ATOM	907	NZ	LYS	L	109	18.009	47.398	33.338	1.00	48.86	L	N
ATOM	908	N	ARG	L	110	22.125	42.691	31.409	1.00	33.89	L	N
ATOM	909	CA	ARG	L	110	22.063	41.786	30.264	1.00	31.44	L	C
ATOM	910	C	ARG	L	110	20.696	41.861	29.596	1.00	28.77	L	C
ATOM	911	O	ARG	L	110	19.690	42.107	30.253	1.00	28.40	L	O
ATOM	912	CB	ARG	L	110	22.334	40.346	30.709	1.00	29.16	L	C
ATOM	913	CG	ARG	L	110	21.206	39.704	31.515	1.00	26.40	L	C
ATOM	914	CD	ARG	L	110	20.133	39.072	30.617	1.00	23.55	L	C
ATOM	915	NE	ARG	L	110	19.049	38.500	31.409	1.00	23.99	L	N
ATOM	916	CZ	ARG	L	110	18.083	39.206	31.993	1.00	26.90	L	C
ATOM	917	NH1	ARG	L	110	18.045	40.529	31.871	1.00	25.76	L	N
ATOM	918	NH2	ARG	L	110	17.163	38.592	32.726	1.00	23.93	L	N
ATOM	919	N	SER	L	111	20.666	41.652	28.287	1.00	27.46	L	N
ATOM	920	CA	SER	L	111	19.416	41.683	27.545	1.00	26.40	L	C
ATOM	921	C	SER	L	111	19.173	40.310	26.925	1.00	25.75	L	C
ATOM	922	O	SER	L	111	20.116	39.578	26.624	1.00	25.72	L	O
ATOM	923	CB	SER	L	111	19.484	42.732	26.442	1.00	23.78	L	C
ATOM	924	OG	SER	L	111	20.407	42.337	25.447	1.00	28.02	L	O
ATOM	925	N	CYS	L	112	17.906	39.962	26.745	1.00	24.32	L	N
ATOM	926	CA	CYS	L	112	17.553	38.682	26.152	1.00	24.98	L	C
ATOM	927	C	CYS	L	112	17.024	38.891	24.742	1.00	24.93	L	C
ATOM	928	O	CYS	L	112	16.341	39.879	24.470	1.00	26.51	L	O
ATOM	929	CB	CYS	L	112	16.480	37.985	26.980	1.00	23.15	L	C
ATOM	930	SG	CYS	L	112	16.932	37.554	28.686	1.00	25.67	L	S
ATOM	931	N	ARG	L	113	17.341	37.961	23.846	1.00	24.52	L	N
ATOM	932	CA	ARG	L	113	16.884	38.042	22.463	1.00	23.03	L	C
ATOM	933	C	ARG	L	113	16.292	36.709	22.021	1.00	22.44	L	C
ATOM	934	O	ARG	L	113	16.260	35.749	22.791	1.00	20.23	L	O
ATOM	935	CB	ARG	L	113	18.038	38.457	21.543	1.00	23.44	L	C
ATOM	936	CG	ARG	L	113	18.470	39.912	21.739	1.00	25.76	L	C
ATOM	937	CD	ARG	L	113	19.706	40.286	20.926	1.00	25.39	L	C
ATOM	938	NE	ARG	L	113	20.882	39.525	21.349	1.00	26.05	L	N
ATOM	939	CZ	ARG	L	113	21.361	38.459	20.712	1.00	22.82	L	C
ATOM	940	NH1	ARG	L	113	20.775	38.019	19.607	1.00	19.33	L	N
ATOM	941	NH2	ARG	L	113	22.421	37.823	21.190	1.00	19.90	L	N
ATOM	942	N	CYS	L	114	15.810	36.656	20.783	1.00	21.91	L	N
ATOM	943	CA	CYS	L	114	15.208	35.439	20.268	1.00	21.36	L	C

ATOM	944	C	CYS	L	114	15.653	35.122	18.847	1.00	20.52	L C
ATOM	945	O	CYS	L	114	16.153	35.979	18.120	1.00	19.97	L O
ATOM	946	CB	CYS	L	114	13.677	35.542	20.296	1.00	20.90	L C
ATOM	947	SG	CYS	L	114	12.941	36.040	21.885	1.00	22.52	L S
ATOM	948	N	HIS	L	115	15.453	33.868	18.469	1.00	20.76	L N
ATOM	949	CA	HIS	L	115	15.786	33.367	17.147	1.00	20.81	L C
ATOM	950	C	HIS	L	115	14.684	33.850	16.199	1.00	21.18	L C
ATOM	951	O	HIS	L	115	13.556	34.098	16.627	1.00	21.61	L O
ATOM	952	CB	HIS	L	115	15.827	31.832	17.207	1.00	20.46	L C
ATOM	953	CG	HIS	L	115	16.269	31.172	15.938	1.00	19.99	L C
ATOM	954	ND1	HIS	L	115	15.455	31.057	14.832	1.00	19.51	L N
ATOM	955	CD2	HIS	L	115	17.442	30.586	15.602	1.00	18.82	L C
ATOM	956	CE1	HIS	L	115	16.107	30.432	13.870	1.00	17.84	L C
ATOM	957	NE2	HIS	L	115	17.315	30.134	14.311	1.00	19.44	L N
ATOM	958	N	GLU	L	116	15.020	34.012	14.925	1.00	21.79	L N
ATOM	959	CA	GLU	L	116	14.050	34.429	13.924	1.00	21.88	L C
ATOM	960	C	GLU	L	116	12.845	33.503	14.053	1.00	20.86	L C
ATOM	961	O	GLU	L	116	13.002	32.306	14.288	1.00	20.19	L O
ATOM	962	CB	GLU	L	116	14.655	34.300	12.522	1.00	25.33	L C
ATOM	963	CG	GLU	L	116	13.663	34.559	11.391	1.00	32.50	L C
ATOM	964	CD	GLU	L	116	14.201	34.154	10.027	1.00	36.87	L C
ATOM	965	OE1	GLU	L	116	13.412	34.107	9.075	1.00	39.33	L O
ATOM	966	OE2	GLU	L	116	15.405	33.890	9.916	1.00	38.85	L O
ATOM	967	N	GLY	L	117	11.646	34.051	13.900	1.00	20.27	L N
ATOM	968	CA	GLY	L	117	10.451	33.236	14.020	1.00	18.99	L C
ATOM	969	C	GLY	L	117	9.860	33.299	15.417	1.00	19.27	L C
ATOM	970	O	GLY	L	117	8.820	32.694	15.688	1.00	19.43	L O
ATOM	971	N	TYR	L	118	10.543	34.018	16.305	1.00	19.01	L N
ATOM	972	CA	TYR	L	118	10.116	34.206	17.689	1.00	19.23	L C
ATOM	973	C	TYR	L	118	10.278	35.692	18.018	1.00	20.14	L C
ATOM	974	O	TYR	L	118	11.012	36.409	17.344	1.00	19.66	L O
ATOM	975	CB	TYR	L	118	10.999	33.417	18.671	1.00	18.12	L C
ATOM	976	CG	TYR	L	118	10.916	31.905	18.602	1.00	15.33	L C
ATOM	977	CD1	TYR	L	118	11.650	31.187	17.658	1.00	15.05	L C
ATOM	978	CD2	TYR	L	118	10.116	31.192	19.499	1.00	13.29	L C
ATOM	979	CE1	TYR	L	118	11.590	29.791	17.607	1.00	14.73	L C
ATOM	980	CE2	TYR	L	118	10.049	29.803	19.457	1.00	14.27	L C
ATOM	981	CZ	TYR	L	118	10.790	29.109	18.507	1.00	15.35	L C
ATOM	982	OH	TYR	L	118	10.736	27.735	18.466	1.00	15.58	L O
ATOM	983	N	SER	L	119	9.595	36.150	19.058	1.00	21.39	L N
ATOM	984	CA	SER	L	119	9.710	37.538	19.481	1.00	23.14	L C
ATOM	985	C	SER	L	119	9.746	37.524	21.002	1.00	21.88	L C
ATOM	986	O	SER	L	119	9.189	36.629	21.632	1.00	23.34	L O
ATOM	987	CB	SER	L	119	8.522	38.364	18.979	1.00	23.84	L C
ATOM	988	OG	SER	L	119	7.312	37.905	19.556	1.00	31.34	L O
ATOM	989	N	LEU	L	120	10.413	38.510	21.585	1.00	23.21	L N
ATOM	990	CA	LEU	L	120	10.544	38.606	23.036	1.00	24.38	L C
ATOM	991	C	LEU	L	120	9.253	39.096	23.683	1.00	26.18	L C
ATOM	992	O	LEU	L	120	8.667	40.081	23.236	1.00	27.69	L O
ATOM	993	CB	LEU	L	120	11.683	39.565	23.389	1.00	23.36	L C
ATOM	994	CG	LEU	L	120	12.119	39.619	24.855	1.00	25.06	L C
ATOM	995	CD1	LEU	L	120	12.801	38.311	25.230	1.00	24.68	L C
ATOM	996	CD2	LEU	L	120	13.080	40.789	25.063	1.00	24.21	L C
ATOM	997	N	LEU	L	121	8.817	38.410	24.736	1.00	26.79	L N
ATOM	998	CA	LEU	L	121	7.600	38.790	25.450	1.00	28.18	L C
ATOM	999	C	LEU	L	121	7.885	39.949	26.402	1.00	29.35	L C

ATOM	1000	O	LEU	L	121	9.039	40.320	26.614	1.00	28.95	L	O
ATOM	1001	CB	LEU	L	121	7.042	37.595	26.235	1.00	26.70	L	C
ATOM	1002	CG	LEU	L	121	6.491	36.417	25.418	1.00	27.20	L	C
ATOM	1003	CD1	LEU	L	121	6.025	35.310	26.348	1.00	27.89	L	C
ATOM	1004	CD2	LEU	L	121	5.335	36.891	24.554	1.00	28.46	L	C
ATOM	1005	N	ALA	L	122	6.825	40.512	26.979	1.00	30.71	L	N
ATOM	1006	CA	ALA	L	122	6.948	41.638	27.903	1.00	30.91	L	C
ATOM	1007	C	ALA	L	122	7.865	41.379	29.097	1.00	30.79	L	C
ATOM	1008	O	ALA	L	122	8.492	42.307	29.607	1.00	32.36	L	O
ATOM	1009	CB	ALA	L	122	5.566	42.058	28.397	1.00	33.12	L	C
ATOM	1010	N	ASP	L	123	7.953	40.131	29.550	1.00	28.66	L	N
ATOM	1011	CA	ASP	L	123	8.811	39.826	30.687	1.00	27.44	L	C
ATOM	1012	C	ASP	L	123	10.301	40.040	30.405	1.00	27.39	L	C
ATOM	1013	O	ASP	L	123	11.123	39.955	31.314	1.00	28.38	L	O
ATOM	1014	CB	ASP	L	123	8.571	38.392	31.189	1.00	27.26	L	C
ATOM	1015	CG	ASP	L	123	8.951	37.324	30.168	1.00	26.53	L	C
ATOM	1016	OD1	ASP	L	123	9.602	37.634	29.173	1.00	25.66	L	O
ATOM	1017	OD2	ASP	L	123	8.595	36.173	30.389	1.00	25.85	L	O
ATOM	1018	N	GLY	L	124	10.645	40.318	29.150	1.00	27.75	L	N
ATOM	1019	CA	GLY	L	124	12.033	40.551	28.789	1.00	27.23	L	C
ATOM	1020	C	GLY	L	124	12.937	39.329	28.721	1.00	28.17	L	C
ATOM	1021	O	GLY	L	124	14.135	39.465	28.460	1.00	27.43	L	O
ATOM	1022	N	VAL	L	125	12.389	38.137	28.943	1.00	28.24	L	N
ATOM	1023	CA	VAL	L	125	13.205	36.920	28.899	1.00	27.90	L	C
ATOM	1024	C	VAL	L	125	12.626	35.779	28.057	1.00	26.61	L	C
ATOM	1025	O	VAL	L	125	13.373	34.954	27.533	1.00	25.92	L	O
ATOM	1026	CB	VAL	L	125	13.476	36.367	30.326	1.00	28.91	L	C
ATOM	1027	CG1	VAL	L	125	14.182	37.421	31.173	1.00	29.31	L	C
ATOM	1028	CG2	VAL	L	125	12.173	35.930	30.980	1.00	27.68	L	C
ATOM	1029	N	SER	L	126	11.304	35.734	27.927	1.00	25.52	L	N
ATOM	1030	CA	SER	L	126	10.639	34.677	27.175	1.00	23.57	L	C
ATOM	1031	C	SER	L	126	10.475	34.989	25.696	1.00	23.79	L	C
ATOM	1032	O	SER	L	126	10.427	36.157	25.294	1.00	21.55	L	O
ATOM	1033	CB	SER	L	126	9.266	34.393	27.788	1.00	23.48	L	C
ATOM	1034	OG	SER	L	126	9.396	34.047	29.157	1.00	24.08	L	O
ATOM	1035	N	CYS	L	127	10.391	33.932	24.890	1.00	21.77	L	N
ATOM	1036	CA	CYS	L	127	10.219	34.070	23.451	1.00	22.08	L	C
ATOM	1037	C	CYS	L	127	8.966	33.324	23.020	1.00	22.86	L	C
ATOM	1038	O	CYS	L	127	8.698	32.214	23.482	1.00	23.36	L	O
ATOM	1039	CB	CYS	L	127	11.431	33.516	22.700	1.00	21.97	L	C
ATOM	1040	SG	CYS	L	127	13.006	34.368	23.044	1.00	21.79	L	S
ATOM	1041	N	THR	L	128	8.197	33.947	22.136	1.00	21.95	L	N
ATOM	1042	CA	THR	L	128	6.967	33.353	21.645	1.00	21.10	L	C
ATOM	1043	C	THR	L	128	7.041	33.249	20.126	1.00	20.42	L	C
ATOM	1044	O	THR	L	128	7.593	34.126	19.458	1.00	18.28	L	O
ATOM	1045	CB	THR	L	128	5.735	34.210	22.063	1.00	21.74	L	C
ATOM	1046	OG1	THR	L	128	4.530	33.513	21.732	1.00	22.91	L	O
ATOM	1047	CG2	THR	L	128	5.743	35.554	21.353	1.00	18.95	L	C
ATOM	1048	N	PRO	L	129	6.497	32.162	19.559	1.00	21.27	L	N
ATOM	1049	CA	PRO	L	129	6.514	31.960	18.107	1.00	22.20	L	C
ATOM	1050	C	PRO	L	129	5.713	33.026	17.363	1.00	23.45	L	C
ATOM	1051	O	PRO	L	129	4.621	33.394	17.786	1.00	25.63	L	O
ATOM	1052	CB	PRO	L	129	5.891	30.572	17.943	1.00	22.20	L	C
ATOM	1053	CG	PRO	L	129	6.213	29.888	19.247	1.00	21.77	L	C
ATOM	1054	CD	PRO	L	129	5.938	30.984	20.243	1.00	20.67	L	C
ATOM	1055	N	THR	L	130	6.260	33.528	16.262	1.00	23.88	L	N

ATOM	1056	CA	THR	L	130	5.556	34.525	15.465	1.00	25.00	L	C
ATOM	1057	C	THR	L	130	5.164	33.923	14.122	1.00	26.32	L	C
ATOM	1058	O	THR	L	130	4.762	34.639	13.206	1.00	27.47	L	O
ATOM	1059	CB	THR	L	130	6.411	35.774	15.205	1.00	25.51	L	C
ATOM	1060	OG1	THR	L	130	7.591	35.404	14.486	1.00	27.07	L	O
ATOM	1061	CG2	THR	L	130	6.789	36.443	16.513	1.00	27.60	L	C
ATOM	1062	N	VAL	L	131	5.299	32.601	14.014	1.00	24.93	L	N
ATOM	1063	CA	VAL	L	131	4.942	31.870	12.807	1.00	23.51	L	C
ATOM	1064	C	VAL	L	131	4.271	30.565	13.218	1.00	24.02	L	C
ATOM	1065	O	VAL	L	131	4.369	30.139	14.372	1.00	22.94	L	O
ATOM	1066	CB	VAL	L	131	6.178	31.541	11.930	1.00	25.15	L	C
ATOM	1067	CG1	VAL	L	131	6.844	32.831	11.469	1.00	24.40	L	C
ATOM	1068	CG2	VAL	L	131	7.163	30.673	12.705	1.00	23.42	L	C
ATOM	1069	N	GLU	L	132	3.589	29.937	12.268	1.00	22.59	L	N
ATOM	1070	CA	GLU	L	132	2.888	28.690	12.518	1.00	22.16	L	C
ATOM	1071	C	GLU	L	132	3.840	27.537	12.828	1.00	20.71	L	C
ATOM	1072	O	GLU	L	132	3.567	26.720	13.711	1.00	20.40	L	O
ATOM	1073	CB	GLU	L	132	2.004	28.340	11.308	1.00	22.29	L	C
ATOM	1074	CG	GLU	L	132	1.352	26.972	11.390	1.00	27.79	L	C
ATOM	1075	CD	GLU	L	132	0.327	26.730	10.286	1.00	29.81	L	C
ATOM	1076	OE1	GLU	L	132	0.498	27.265	9.196	1.00	30.53	L	O
ATOM	1077	OE2	GLU	L	132	-0.636	25.985	10.526	1.00	30.39	L	O
ATOM	1078	N	TYR	L	133	4.955	27.473	12.109	1.00	19.60	L	N
ATOM	1079	CA	TYR	L	133	5.930	26.404	12.317	1.00	17.97	L	C
ATOM	1080	C	TYR	L	133	7.320	26.925	12.654	1.00	16.71	L	C
ATOM	1081	O	TYR	L	133	8.236	26.860	11.834	1.00	16.11	L	O
ATOM	1082	CB	TYR	L	133	5.998	25.511	11.077	1.00	17.19	L	C
ATOM	1083	CG	TYR	L	133	4.737	24.717	10.874	1.00	19.02	L	C
ATOM	1084	CD1	TYR	L	133	4.412	23.673	11.735	1.00	16.92	L	C
ATOM	1085	CD2	TYR	L	133	3.833	25.049	9.862	1.00	19.13	L	C
ATOM	1086	CE1	TYR	L	133	3.220	22.978	11.602	1.00	18.85	L	C
ATOM	1087	CE2	TYR	L	133	2.632	24.358	9.719	1.00	18.71	L	C
ATOM	1088	CZ	TYR	L	133	2.335	23.327	10.594	1.00	19.77	L	C
ATOM	1089	OH	TYR	L	133	1.159	22.640	10.467	1.00	20.62	L	O
ATOM	1090	N	PRO	L	134	7.499	27.440	13.878	1.00	15.85	L	N
ATOM	1091	CA	PRO	L	134	8.804	27.963	14.291	1.00	15.14	L	C
ATOM	1092	C	PRO	L	134	9.807	26.814	14.412	1.00	15.88	L	C
ATOM	1093	O	PRO	L	134	9.419	25.677	14.677	1.00	17.59	L	O
ATOM	1094	CB	PRO	L	134	8.497	28.623	15.630	1.00	13.01	L	C
ATOM	1095	CG	PRO	L	134	7.444	27.730	16.198	1.00	13.89	L	C
ATOM	1096	CD	PRO	L	134	6.543	27.455	15.002	1.00	15.08	L	C
ATOM	1097	N	CYS	L	135	11.086	27.108	14.206	1.00	15.52	L	N
ATOM	1098	CA	CYS	L	135	12.125	26.084	14.291	1.00	14.64	L	C
ATOM	1099	C	CYS	L	135	12.228	25.562	15.714	1.00	14.59	L	C
ATOM	1100	O	CYS	L	135	11.874	26.263	16.663	1.00	12.74	L	O
ATOM	1101	CB	CYS	L	135	13.486	26.660	13.875	1.00	13.94	L	C
ATOM	1102	SG	CYS	L	135	14.133	27.949	14.997	1.00	16.77	L	S
ATOM	1103	N	GLY	L	136	12.709	24.328	15.852	1.00	14.02	L	N
ATOM	1104	CA	GLY	L	136	12.902	23.737	17.167	1.00	14.41	L	C
ATOM	1105	C	GLY	L	136	11.682	23.301	17.957	1.00	15.69	L	C
ATOM	1106	O	GLY	L	136	11.810	22.917	19.119	1.00	16.17	L	O
ATOM	1107	N	LYS	L	137	10.501	23.358	17.352	1.00	15.50	L	N
ATOM	1108	CA	LYS	L	137	9.284	22.935	18.036	1.00	17.12	L	C
ATOM	1109	C	LYS	L	137	8.701	21.730	17.309	1.00	17.03	L	C
ATOM	1110	O	LYS	L	137	8.709	21.669	16.077	1.00	17.59	L	O
ATOM	1111	CB	LYS	L	137	8.248	24.063	18.058	1.00	16.09	L	C

ATOM	1112	CG	LYS	L	137	8.085	24.783	19.382	1.00	20.53	L C
ATOM	1113	CD	LYS	L	137	9.354	25.441	19.855	1.00	23.98	L C
ATOM	1114	CE	LYS	L	137	9.056	26.486	20.935	1.00	26.98	L C
ATOM	1115	NZ	LYS	L	137	8.408	25.912	22.147	1.00	27.12	L N
ATOM	1116	N	ILE	L	138	8.191	20.780	18.082	1.00	16.47	L N
ATOM	1117	CA	ILE	L	138	7.598	19.568	17.536	1.00	16.51	L C
ATOM	1118	C	ILE	L	138	6.072	19.699	17.623	1.00	17.05	L C
ATOM	1119	O	ILE	L	138	5.479	19.442	18.665	1.00	17.09	L O
ATOM	1120	CB	ILE	L	138	8.091	18.340	18.332	1.00	16.51	L C
ATOM	1121	CG1	ILE	L	138	9.630	18.329	18.335	1.00	14.34	L C
ATOM	1122	CG2	ILE	L	138	7.534	17.048	17.713	1.00	15.08	L C
ATOM	1123	CD1	ILE	L	138	10.268	17.188	19.119	1.00	12.57	L C
ATOM	1124	N	PRO	L	139	5.421	20.096	16.514	1.00	18.81	L N
ATOM	1125	CA	PRO	L	139	3.963	20.284	16.436	1.00	19.59	L C
ATOM	1126	C	PRO	L	139	3.016	19.231	17.016	1.00	19.28	L C
ATOM	1127	O	PRO	L	139	2.065	19.588	17.708	1.00	20.94	L O
ATOM	1128	CB	PRO	L	139	3.718	20.548	14.943	1.00	19.14	L C
ATOM	1129	CG	PRO	L	139	4.902	19.948	14.273	1.00	22.59	L C
ATOM	1130	CD	PRO	L	139	6.034	20.304	15.195	1.00	18.46	L C
ATOM	1131	N	ILE	L	140	3.249	17.948	16.764	1.00	18.16	L N
ATOM	1132	CA	ILE	L	140	2.334	16.952	17.317	1.00	19.99	L C
ATOM	1133	C	ILE	L	140	2.398	16.843	18.844	1.00	21.32	L C
ATOM	1134	O	ILE	L	140	1.550	16.194	19.454	1.00	21.50	L O
ATOM	1135	CB	ILE	L	140	2.549	15.544	16.711	1.00	20.09	L C
ATOM	1136	CG1	ILE	L	140	3.953	15.034	17.030	1.00	18.72	L C
ATOM	1137	CG2	ILE	L	140	2.294	15.586	15.197	1.00	21.80	L C
ATOM	1138	CD1	ILE	L	140	4.178	13.596	16.611	1.00	20.33	L C
ATOM	1139	N	LEU	L	141	3.397	17.475	19.458	1.00	21.36	L N
ATOM	1140	CA	LEU	L	141	3.531	17.458	20.912	1.00	23.29	L C
ATOM	1141	C	LEU	L	141	3.115	18.806	21.505	1.00	25.19	L C
ATOM	1142	O	LEU	L	141	2.965	18.942	22.716	1.00	25.84	L O
ATOM	1143	CB	LEU	L	141	4.975	17.144	21.315	1.00	21.25	L C
ATOM	1144	CG	LEU	L	141	5.601	15.886	20.705	1.00	21.10	L C
ATOM	1145	CD1	LEU	L	141	6.998	15.706	21.268	1.00	19.02	L C
ATOM	1146	CD2	LEU	L	141	4.732	14.665	20.998	1.00	19.82	L C
ATOM	1147	N	GLU	L	142	2.936	19.804	20.648	1.00	29.07	L N
ATOM	1148	CA	GLU	L	142	2.534	21.131	21.093	1.00	32.74	L C
ATOM	1149	C	GLU	L	142	1.011	21.223	21.174	1.00	35.09	L C
ATOM	1150	O	GLU	L	142	0.514	21.605	22.226	1.00	37.74	L O
ATOM	1151	CB	GLU	L	142	3.067	22.194	20.130	1.00	32.55	L C
ATOM	1152	CG	GLU	L	142	4.577	22.381	20.166	1.00	35.63	L C
ATOM	1153	CD	GLU	L	142	5.062	23.007	21.462	1.00	37.38	L C
ATOM	1154	OE1	GLU	L	142	4.494	24.028	21.871	1.00	39.09	L O
ATOM	1155	OE2	GLU	L	142	6.008	22.486	22.053	1.00	36.36	L O
ATOM	1156	OT	GLU	L	142	0.349	20.913	20.180	1.00	36.04	L O
ATOM	1157	N	ILE	H	16	21.992	3.783	14.153	1.00	14.10	H N
ATOM	1158	CA	ILE	H	16	21.860	4.032	15.614	1.00	13.89	H C
ATOM	1159	C	ILE	H	16	21.875	2.706	16.373	1.00	14.85	H C
ATOM	1160	O	ILE	H	16	21.043	1.834	16.132	1.00	14.89	H O
ATOM	1161	CB	ILE	H	16	20.534	4.767	15.944	1.00	13.63	H C
ATOM	1162	CG1	ILE	H	16	20.451	6.095	15.183	1.00	12.69	H C
ATOM	1163	CG2	ILE	H	16	20.436	4.989	17.450	1.00	11.22	H C
ATOM	1164	CD1	ILE	H	16	21.567	7.092	15.493	1.00	10.60	H C
ATOM	1165	N	VAL	H	17	22.830	2.564	17.285	1.00	16.19	H N
ATOM	1166	CA	VAL	H	17	22.967	1.358	18.092	1.00	16.46	H C
ATOM	1167	C	VAL	H	17	22.445	1.593	19.504	1.00	15.78	H C

ATOM	1168	O	VAL	H	17	22.861	2.536	20.178	1.00	14.50	H	O
ATOM	1169	CB	VAL	H	17	24.451	0.918	18.195	1.00	17.79	H	C
ATOM	1170	CG1	VAL	H	17	24.581	-0.259	19.145	1.00	19.06	H	C
ATOM	1171	CG2	VAL	H	17	24.977	0.529	16.826	1.00	19.20	H	C
ATOM	1172	N	GLY	H	18	21.532	0.735	19.950	1.00	15.38	H	N
ATOM	1173	CA	GLY	H	18	20.990	0.876	21.292	1.00	13.01	H	C
ATOM	1174	C	GLY	H	18	19.982	1.998	21.472	1.00	12.80	H	C
ATOM	1175	O	GLY	H	18	19.768	2.468	22.583	1.00	11.44	H	O
ATOM	1176	N	GLY	H	19	19.365	2.436	20.384	1.00	11.70	H	N
ATOM	1177	CA	GLY	H	19	18.368	3.487	20.483	1.00	13.29	H	C
ATOM	1178	C	GLY	H	19	16.964	2.926	20.333	1.00	13.92	H	C
ATOM	1179	O	GLY	H	19	16.731	1.736	20.540	1.00	13.45	H	O
ATOM	1180	N	LYS	H	20	16.016	3.783	19.977	1.00	15.81	H	N
ATOM	1181	CA	LYS	H	20	14.644	3.341	19.788	1.00	17.79	H	C
ATOM	1182	C	LYS	H	20	14.064	4.033	18.567	1.00	16.64	H	C
ATOM	1183	O	LYS	H	20	14.683	4.935	18.009	1.00	13.94	H	O
ATOM	1184	CB	LYS	H	20	13.794	3.668	21.024	1.00	19.44	H	C
ATOM	1185	CG	LYS	H	20	14.312	3.043	22.317	1.00	26.17	H	C
ATOM	1186	CD	LYS	H	20	13.307	3.186	23.450	1.00	29.52	H	C
ATOM	1187	CE	LYS	H	20	13.918	2.824	24.806	1.00	32.88	H	C
ATOM	1188	NZ	LYS	H	20	14.426	1.423	24.867	1.00	33.23	H	N
ATOM	1189	N	VAL	H	21	12.881	3.601	18.148	1.00	13.39	H	N
ATOM	1190	CA	VAL	H	21	12.228	4.213	17.007	1.00	14.10	H	C
ATOM	1191	C	VAL	H	21	11.729	5.610	17.393	1.00	15.28	H	C
ATOM	1192	O	VAL	H	21	11.136	5.796	18.459	1.00	15.43	H	O
ATOM	1193	CB	VAL	H	21	11.022	3.356	16.530	1.00	14.85	H	C
ATOM	1194	CG1	VAL	H	21	10.233	4.104	15.446	1.00	15.73	H	C
ATOM	1195	CG2	VAL	H	21	11.517	2.018	15.982	1.00	13.11	H	C
ATOM	1196	N	CYS	H	22	11.992	6.595	16.542	1.00	14.61	H	N
ATOM	1197	CA	CYS	H	22	11.518	7.944	16.805	1.00	15.34	H	C
ATOM	1198	C	CYS	H	22	10.063	7.948	16.362	1.00	15.49	H	C
ATOM	1199	O	CYS	H	22	9.779	7.785	15.176	1.00	16.18	H	O
ATOM	1200	CB	CYS	H	22	12.279	8.984	15.976	1.00	13.94	H	C
ATOM	1201	SG	CYS	H	22	11.768	10.666	16.438	1.00	14.65	H	S
ATOM	1202	N	PRO	H	23	9.120	8.127	17.301	1.00	16.39	H	N
ATOM	1203	CA	PRO	H	23	7.710	8.134	16.898	1.00	16.45	H	C
ATOM	1204	C	PRO	H	23	7.491	9.096	15.733	1.00	16.91	H	C
ATOM	1205	O	PRO	H	23	7.995	10.220	15.746	1.00	17.56	H	O
ATOM	1206	CB	PRO	H	23	6.993	8.577	18.171	1.00	16.38	H	C
ATOM	1207	CG	PRO	H	23	7.863	7.993	19.250	1.00	16.66	H	C
ATOM	1208	CD	PRO	H	23	9.251	8.348	18.753	1.00	15.94	H	C
ATOM	1209	N	LYS	H	24	6.746	8.647	14.730	1.00	16.37	H	N
ATOM	1210	CA	LYS	H	24	6.464	9.456	13.549	1.00	16.46	H	C
ATOM	1211	C	LYS	H	24	6.117	10.895	13.915	1.00	15.64	H	C
ATOM	1212	O	LYS	H	24	5.211	11.145	14.707	1.00	17.81	H	O
ATOM	1213	CB	LYS	H	24	5.314	8.836	12.757	1.00	17.93	H	C
ATOM	1214	CG	LYS	H	24	5.122	9.431	11.369	1.00	19.08	H	C
ATOM	1215	CD	LYS	H	24	3.979	8.750	10.648	1.00	19.14	H	C
ATOM	1216	CE	LYS	H	24	4.144	8.839	9.143	1.00	23.91	H	C
ATOM	1217	NZ	LYS	H	24	4.196	10.230	8.631	1.00	20.21	H	N
ATOM	1218	N	GLY	H	25	6.845	11.842	13.340	1.00	14.95	H	N
ATOM	1219	CA	GLY	H	25	6.586	13.239	13.638	1.00	14.04	H	C
ATOM	1220	C	GLY	H	25	7.403	13.847	14.769	1.00	13.80	H	C
ATOM	1221	O	GLY	H	25	7.427	15.068	14.909	1.00	13.20	H	O
ATOM	1222	N	GLU	H	26	8.076	13.026	15.573	1.00	13.01	H	N
ATOM	1223	CA	GLU	H	26	8.874	13.560	16.683	1.00	15.70	H	C

ATOM	1224	C	GLU	H	26	10.331	13.897	16.348	1.00	15.14	H	C
ATOM	1225	O	GLU	H	26	11.078	14.380	17.196	1.00	15.40	H	O
ATOM	1226	CB	GLU	H	26	8.789	12.625	17.898	1.00	15.76	H	C
ATOM	1227	CG	GLU	H	26	7.483	12.816	18.668	1.00	19.10	H	C
ATOM	1228	CD	GLU	H	26	7.346	11.908	19.874	1.00	21.34	H	C
ATOM	1229	OE1	GLU	H	26	8.322	11.730	20.591	1.00	22.66	H	O
ATOM	1230	OE2	GLU	H	26	6.249	11.395	20.097	1.00	22.32	H	O
ATOM	1231	N	CYS	H	27	10.716	13.641	15.103	1.00	15.31	H	N
ATOM	1232	CA	CYS	H	27	12.048	13.958	14.582	1.00	14.35	H	C
ATOM	1233	C	CYS	H	27	11.749	14.611	13.217	1.00	14.44	H	C
ATOM	1234	O	CYS	H	27	12.256	14.170	12.188	1.00	15.00	H	O
ATOM	1235	CB	CYS	H	27	12.873	12.663	14.404	1.00	16.45	H	C
ATOM	1236	SG	CYS	H	27	13.342	11.868	15.982	1.00	16.62	H	S
ATOM	1237	N	PRO	H	28	10.935	15.693	13.204	1.00	12.78	H	N
ATOM	1238	CA	PRO	H	28	10.550	16.393	11.972	1.00	12.72	H	C
ATOM	1239	C	PRO	H	28	11.596	17.135	11.142	1.00	13.51	H	C
ATOM	1240	O	PRO	H	28	11.334	17.470	9.989	1.00	14.79	H	O
ATOM	1241	CB	PRO	H	28	9.414	17.300	12.443	1.00	10.56	H	C
ATOM	1242	CG	PRO	H	28	9.872	17.708	13.785	1.00	12.39	H	C
ATOM	1243	CD	PRO	H	28	10.409	16.411	14.382	1.00	13.71	H	C
ATOM	1244	N	TRP	H	29	12.763	17.403	11.715	1.00	13.66	H	N
ATOM	1245	CA	TRP	H	29	13.837	18.072	10.981	1.00	12.45	H	C
ATOM	1246	C	TRP	H	29	14.801	17.058	10.344	1.00	13.04	H	C
ATOM	1247	O	TRP	H	29	15.741	17.447	9.651	1.00	12.14	H	O
ATOM	1248	CB	TRP	H	29	14.622	19.019	11.905	1.00	10.27	H	C
ATOM	1249	CG	TRP	H	29	14.719	18.544	13.333	1.00	10.51	H	C
ATOM	1250	CD1	TRP	H	29	15.510	17.540	13.818	1.00	9.50	H	C
ATOM	1251	CD2	TRP	H	29	13.935	19.009	14.441	1.00	9.92	H	C
ATOM	1252	NE1	TRP	H	29	15.261	17.347	15.159	1.00	9.49	H	N
ATOM	1253	CE2	TRP	H	29	14.299	18.235	15.566	1.00	9.72	H	C
ATOM	1254	CE3	TRP	H	29	12.961	20.004	14.590	1.00	8.87	H	C
ATOM	1255	CZ2	TRP	H	29	13.717	18.424	16.824	1.00	9.39	H	C
ATOM	1256	CZ3	TRP	H	29	12.381	20.193	15.842	1.00	9.88	H	C
ATOM	1257	CH2	TRP	H	29	12.763	19.404	16.944	1.00	9.90	H	C
ATOM	1258	N	GLN	H	30	14.566	15.765	10.573	1.00	12.37	H	N
ATOM	1259	CA	GLN	H	30	15.427	14.723	10.011	1.00	11.48	H	C
ATOM	1260	C	GLN	H	30	15.253	14.653	8.496	1.00	11.76	H	C
ATOM	1261	O	GLN	H	30	14.128	14.696	7.987	1.00	10.36	H	O
ATOM	1262	CB	GLN	H	30	15.090	13.363	10.622	1.00	12.28	H	C
ATOM	1263	CG	GLN	H	30	15.832	12.180	9.982	1.00	13.59	H	C
ATOM	1264	CD	GLN	H	30	17.291	12.090	10.401	1.00	11.47	H	C
ATOM	1265	OE1	GLN	H	30	18.171	11.810	9.587	1.00	15.48	H	O
ATOM	1266	NE2	GLN	H	30	17.548	12.306	11.675	1.00	9.74	H	N
ATOM	1267	N	VAL	H	31	16.372	14.542	7.785	1.00	10.70	H	N
ATOM	1268	CA	VAL	H	31	16.369	14.468	6.327	1.00	7.92	H	C
ATOM	1269	C	VAL	H	31	16.999	13.155	5.865	1.00	9.83	H	C
ATOM	1270	O	VAL	H	31	17.922	12.641	6.501	1.00	12.57	H	O
ATOM	1271	CB	VAL	H	31	17.194	15.635	5.698	1.00	11.09	H	C
ATOM	1272	CG1	VAL	H	31	17.177	15.534	4.167	1.00	9.42	H	C
ATOM	1273	CG2	VAL	H	31	16.641	16.996	6.142	1.00	7.29	H	C
ATOM	1274	N	LEU	H	32	16.481	12.600	4.773	1.00	10.90	H	N
ATOM	1275	CA	LEU	H	32	17.034	11.384	4.193	1.00	10.82	H	C
ATOM	1276	C	LEU	H	32	17.618	11.785	2.847	1.00	12.58	H	C
ATOM	1277	O	LEU	H	32	16.902	12.294	1.984	1.00	13.53	H	O
ATOM	1278	CB	LEU	H	32	15.951	10.330	3.967	1.00	10.99	H	C
ATOM	1279	CG	LEU	H	32	16.394	9.157	3.082	1.00	12.15	H	C

ATOM	1280	CD1	LEU	H	32	17.496	8.366	3.774	1.00	10.81	H	C
ATOM	1281	CD2	LEU	H	32	15.200	8.251	2.796	1.00	12.95	H	C
ATOM	1282	N	LEU	H	33	18.916	11.575	2.669	1.00	11.95	H	N
ATOM	1283	CA	LEU	H	33	19.566	11.921	1.411	1.00	13.59	H	C
ATOM	1284	C	LEU	H	33	19.777	10.668	0.585	1.00	14.19	H	C
ATOM	1285	O	LEU	H	33	20.252	9.649	1.090	1.00	13.59	H	O
ATOM	1286	CB	LEU	H	33	20.915	12.611	1.663	1.00	13.43	H	C
ATOM	1287	CG	LEU	H	33	20.843	13.953	2.401	1.00	13.16	H	C
ATOM	1288	CD1	LEU	H	33	22.246	14.429	2.718	1.00	11.72	H	C
ATOM	1289	CD2	LEU	H	33	20.103	14.981	1.546	1.00	14.08	H	C
ATOM	1290	N	LEU	H	34	19.423	10.757	-0.691	1.00	16.19	H	N
ATOM	1291	CA	LEU	H	34	19.553	9.636	-1.611	1.00	17.59	H	C
ATOM	1292	C	LEU	H	34	20.384	10.026	-2.826	1.00	18.00	H	C
ATOM	1293	O	LEU	H	34	20.372	11.177	-3.261	1.00	18.90	H	O
ATOM	1294	CB	LEU	H	34	18.165	9.184	-2.086	1.00	19.63	H	C
ATOM	1295	CG	LEU	H	34	17.092	8.859	-1.033	1.00	21.00	H	C
ATOM	1296	CD1	LEU	H	34	15.741	8.708	-1.712	1.00	22.40	H	C
ATOM	1297	CD2	LEU	H	34	17.457	7.595	-0.288	1.00	21.37	H	C
ATOM	1298	N	VAL	H	35	21.126	9.066	-3.357	1.00	19.10	H	N
ATOM	1299	CA	VAL	H	35	21.915	9.294	-4.553	1.00	20.91	H	C
ATOM	1300	C	VAL	H	35	21.484	8.174	-5.494	1.00	21.66	H	C
ATOM	1301	O	VAL	H	35	21.512	7.004	-5.124	1.00	22.02	H	O
ATOM	1302	CB	VAL	H	35	23.438	9.229	-4.275	1.00	21.22	H	C
ATOM	1303	CG1	VAL	H	35	23.846	7.837	-3.828	1.00	23.40	H	C
ATOM	1304	CG2	VAL	H	35	24.201	9.641	-5.516	1.00	23.57	H	C
ATOM	1305	N	ASN	H	37	21.049	8.539	-6.694	1.00	22.76	H	N
ATOM	1306	CA	ASN	H	37	20.575	7.557	-7.668	1.00	24.27	H	C
ATOM	1307	C	ASN	H	37	19.473	6.695	-7.049	1.00	24.89	H	C
ATOM	1308	O	ASN	H	37	19.385	5.502	-7.333	1.00	25.83	H	O
ATOM	1309	CB	ASN	H	37	21.721	6.650	-8.130	1.00	25.18	H	C
ATOM	1310	CG	ASN	H	37	22.904	7.428	-8.674	1.00	27.92	H	C
ATOM	1311	OD1	ASN	H	37	22.757	8.269	-9.563	1.00	26.24	H	O
ATOM	1312	ND2	ASN	H	37	24.090	7.144	-8.142	1.00	29.79	H	N
ATOM	1313	N	GLY	H	38	18.645	7.300	-6.198	1.00	25.00	H	N
ATOM	1314	CA	GLY	H	38	17.568	6.575	-5.545	1.00	23.40	H	C
ATOM	1315	C	GLY	H	38	17.977	5.678	-4.386	1.00	23.72	H	C
ATOM	1316	O	GLY	H	38	17.126	5.033	-3.777	1.00	25.41	H	O
ATOM	1317	N	ALA	H	39	19.268	5.630	-4.070	1.00	22.78	H	N
ATOM	1318	CA	ALA	H	39	19.757	4.791	-2.981	1.00	22.39	H	C
ATOM	1319	C	ALA	H	39	20.050	5.607	-1.724	1.00	22.79	H	C
ATOM	1320	O	ALA	H	39	20.450	6.767	-1.807	1.00	23.53	H	O
ATOM	1321	CB	ALA	H	39	21.014	4.056	-3.419	1.00	20.94	H	C
ATOM	1322	N	GLN	H	40	19.848	4.993	-0.562	1.00	22.25	H	N
ATOM	1323	CA	GLN	H	40	20.098	5.658	0.714	1.00	22.90	H	C
ATOM	1324	C	GLN	H	40	21.574	6.042	0.824	1.00	22.41	H	C
ATOM	1325	O	GLN	H	40	22.456	5.192	0.716	1.00	22.51	H	O
ATOM	1326	CB	GLN	H	40	19.720	4.730	1.871	1.00	22.59	H	C
ATOM	1327	CG	GLN	H	40	19.763	5.385	3.247	1.00	25.18	H	C
ATOM	1328	CD	GLN	H	40	19.409	4.415	4.363	1.00	26.21	H	C
ATOM	1329	OE1	GLN	H	40	18.430	3.676	4.270	1.00	26.38	H	O
ATOM	1330	NE2	GLN	H	40	20.198	4.421	5.430	1.00	26.47	H	N
ATOM	1331	N	LEU	H	41	21.837	7.324	1.052	1.00	21.11	H	N
ATOM	1332	CA	LEU	H	41	23.206	7.816	1.164	1.00	19.35	H	C
ATOM	1333	C	LEU	H	41	23.585	8.285	2.570	1.00	18.35	H	C
ATOM	1334	O	LEU	H	41	24.552	7.800	3.152	1.00	18.12	H	O
ATOM	1335	CB	LEU	H	41	23.419	8.978	0.184	1.00	19.30	H	C

ATOM	1336	CG	LEU	H	41	24.745	9.744	0.271	1.00	17.33	H	C
ATOM	1337	CD1	LEU	H	41	25.890	8.880	-0.246	1.00	14.99	H	C
ATOM	1338	CD2	LEU	H	41	24.641	11.016	-0.540	1.00	16.13	H	C
ATOM	1339	N	CYS	H	42	22.816	9.226	3.110	1.00	16.56	H	N
ATOM	1340	CA	CYS	H	42	23.108	9.796	4.421	1.00	15.14	H	C
ATOM	1341	C	CYS	H	42	21.907	10.492	5.033	1.00	13.30	H	C
ATOM	1342	O	CYS	H	42	20.851	10.595	4.418	1.00	12.64	H	O
ATOM	1343	CB	CYS	H	42	24.226	10.844	4.291	1.00	15.11	H	C
ATOM	1344	SG	CYS	H	42	25.929	10.216	4.342	1.00	18.96	H	S
ATOM	1345	N	GLY	H	43	22.101	10.988	6.251	1.00	11.79	H	N
ATOM	1346	CA	GLY	H	43	21.064	11.728	6.932	1.00	9.99	H	C
ATOM	1347	C	GLY	H	43	21.362	13.209	6.753	1.00	10.90	H	C
ATOM	1348	O	GLY	H	43	22.362	13.580	6.138	1.00	12.00	H	O
ATOM	1349	N	GLY	H	44	20.491	14.058	7.281	1.00	11.43	H	N
ATOM	1350	CA	GLY	H	44	20.690	15.493	7.183	1.00	9.27	H	C
ATOM	1351	C	GLY	H	44	19.747	16.195	8.143	1.00	9.66	H	C
ATOM	1352	O	GLY	H	44	18.884	15.553	8.741	1.00	8.35	H	O
ATOM	1353	N	THR	H	45	19.908	17.507	8.293	1.00	10.40	H	N
ATOM	1354	CA	THR	H	45	19.062	18.286	9.186	1.00	10.32	H	C
ATOM	1355	C	THR	H	45	18.500	19.512	8.470	1.00	12.51	H	C
ATOM	1356	O	THR	H	45	19.247	20.315	7.914	1.00	12.61	H	O
ATOM	1357	CB	THR	H	45	19.856	18.781	10.420	1.00	11.05	H	C
ATOM	1358	OG1	THR	H	45	20.468	17.667	11.084	1.00	11.48	H	O
ATOM	1359	CG2	THR	H	45	18.934	19.491	11.399	1.00	9.59	H	C
ATOM	1360	N	LEU	H	46	17.185	19.662	8.475	1.00	12.48	H	N
ATOM	1361	CA	LEU	H	46	16.572	20.824	7.840	1.00	12.20	H	C
ATOM	1362	C	LEU	H	46	16.689	21.980	8.829	1.00	12.78	H	C
ATOM	1363	O	LEU	H	46	16.377	21.818	10.006	1.00	12.83	H	O
ATOM	1364	CB	LEU	H	46	15.090	20.553	7.558	1.00	14.68	H	C
ATOM	1365	CG	LEU	H	46	14.273	21.611	6.805	1.00	13.62	H	C
ATOM	1366	CD1	LEU	H	46	14.639	21.570	5.321	1.00	12.45	H	C
ATOM	1367	CD2	LEU	H	46	12.783	21.326	6.973	1.00	12.25	H	C
ATOM	1368	N	ILE	H	47	17.163	23.135	8.377	1.00	12.00	H	N
ATOM	1369	CA	ILE	H	47	17.252	24.288	9.275	1.00	13.26	H	C
ATOM	1370	C	ILE	H	47	16.475	25.470	8.686	1.00	15.67	H	C
ATOM	1371	O	ILE	H	47	16.356	26.523	9.312	1.00	17.65	H	O
ATOM	1372	CB	ILE	H	47	18.727	24.714	9.552	1.00	11.94	H	C
ATOM	1373	CG1	ILE	H	47	19.427	25.098	8.249	1.00	12.91	H	C
ATOM	1374	CG2	ILE	H	47	19.476	23.575	10.248	1.00	10.11	H	C
ATOM	1375	CD1	ILE	H	47	20.815	25.683	8.455	1.00	13.22	H	C
ATOM	1376	N	ASN	H	48	15.944	25.264	7.481	1.00	17.72	H	N
ATOM	1377	CA	ASN	H	48	15.158	26.245	6.738	1.00	21.07	H	C
ATOM	1378	C	ASN	H	48	14.312	25.485	5.728	1.00	20.14	H	C
ATOM	1379	O	ASN	H	48	14.506	24.288	5.536	1.00	20.62	H	O
ATOM	1380	CB	ASN	H	48	16.071	27.199	5.965	1.00	27.12	H	C
ATOM	1381	CG	ASN	H	48	16.437	28.416	6.759	1.00	32.69	H	C
ATOM	1382	OD1	ASN	H	48	15.566	29.193	7.156	1.00	37.95	H	O
ATOM	1383	ND2	ASN	H	48	17.729	28.600	6.998	1.00	33.59	H	N
ATOM	1384	N	THR	H	49	13.387	26.176	5.069	1.00	18.81	H	N
ATOM	1385	CA	THR	H	49	12.562	25.521	4.055	1.00	19.09	H	C
ATOM	1386	C	THR	H	49	13.421	25.187	2.838	1.00	18.19	H	C
ATOM	1387	O	THR	H	49	13.065	24.315	2.044	1.00	19.04	H	O
ATOM	1388	CB	THR	H	49	11.400	26.419	3.570	1.00	16.92	H	C
ATOM	1389	OG1	THR	H	49	11.932	27.615	2.989	1.00	18.22	H	O
ATOM	1390	CG2	THR	H	49	10.485	26.780	4.716	1.00	17.02	H	C
ATOM	1391	N	ILE	H	50	14.559	25.871	2.707	1.00	18.59	H	N

ATOM	1392	CA	ILE	H	50	15.469	25.674	1.576	1.00	18.42	H	C
ATOM	1393	C	ILE	H	50	16.841	25.067	1.907	1.00	18.14	H	C
ATOM	1394	O	ILE	H	50	17.499	24.507	1.025	1.00	17.04	H	O
ATOM	1395	CB	ILE	H	50	15.694	27.030	0.841	1.00	22.10	H	C
ATOM	1396	CG1	ILE	H	50	14.481	27.357	-0.030	1.00	21.65	H	C
ATOM	1397	CG2	ILE	H	50	16.953	26.987	-0.022	1.00	23.17	H	C
ATOM	1398	CD1	ILE	H	50	14.338	26.454	-1.235	1.00	23.27	H	C
ATOM	1399	N	TRP	H	51	17.274	25.160	3.161	1.00	16.05	H	N
ATOM	1400	CA	TRP	H	51	18.592	24.655	3.528	1.00	15.56	H	C
ATOM	1401	C	TRP	H	51	18.659	23.436	4.438	1.00	15.82	H	C
ATOM	1402	O	TRP	H	51	17.932	23.321	5.424	1.00	16.64	H	O
ATOM	1403	CB	TRP	H	51	19.423	25.775	4.149	1.00	16.33	H	C
ATOM	1404	CG	TRP	H	51	19.593	26.967	3.254	1.00	15.89	H	C
ATOM	1405	CD1	TRP	H	51	18.847	28.111	3.261	1.00	15.94	H	C
ATOM	1406	CD2	TRP	H	51	20.576	27.134	2.224	1.00	15.03	H	C
ATOM	1407	NE1	TRP	H	51	19.306	28.982	2.302	1.00	16.22	H	N
ATOM	1408	CE2	TRP	H	51	20.367	28.409	1.651	1.00	16.38	H	C
ATOM	1409	CE3	TRP	H	51	21.615	26.330	1.730	1.00	16.52	H	C
ATOM	1410	CZ2	TRP	H	51	21.163	28.904	0.606	1.00	16.04	H	C
ATOM	1411	CZ3	TRP	H	51	22.405	26.822	0.690	1.00	16.73	H	C
ATOM	1412	CH2	TRP	H	51	22.173	28.100	0.142	1.00	16.02	H	C
ATOM	1413	N	VAL	H	52	19.571	22.536	4.091	1.00	14.41	H	N
ATOM	1414	CA	VAL	H	52	19.794	21.306	4.831	1.00	12.34	H	C
ATOM	1415	C	VAL	H	52	21.270	21.211	5.218	1.00	11.65	H	C
ATOM	1416	O	VAL	H	52	22.136	21.461	4.391	1.00	9.66	H	O
ATOM	1417	CB	VAL	H	52	19.440	20.073	3.957	1.00	11.76	H	C
ATOM	1418	CG1	VAL	H	52	19.909	18.800	4.632	1.00	8.59	H	C
ATOM	1419	CG2	VAL	H	52	17.935	20.022	3.700	1.00	12.24	H	C
ATOM	1420	N	VAL	H	53	21.549	20.869	6.474	1.00	11.58	H	N
ATOM	1421	CA	VAL	H	53	22.925	20.706	6.944	1.00	11.42	H	C
ATOM	1422	C	VAL	H	53	23.198	19.206	7.023	1.00	11.69	H	C
ATOM	1423	O	VAL	H	53	22.431	18.470	7.629	1.00	12.13	H	O
ATOM	1424	CB	VAL	H	53	23.141	21.326	8.357	1.00	11.61	H	C
ATOM	1425	CG1	VAL	H	53	24.522	20.923	8.910	1.00	6.99	H	C
ATOM	1426	CG2	VAL	H	53	23.037	22.850	8.284	1.00	9.62	H	C
ATOM	1427	N	SER	H	54	24.280	18.757	6.397	1.00	11.72	H	N
ATOM	1428	CA	SER	H	54	24.642	17.343	6.414	1.00	10.64	H	C
ATOM	1429	C	SER	H	54	26.150	17.233	6.651	1.00	11.91	H	C
ATOM	1430	O	SER	H	54	26.770	18.184	7.134	1.00	12.10	H	O
ATOM	1431	CB	SER	H	54	24.256	16.687	5.082	1.00	10.42	H	C
ATOM	1432	OG	SER	H	54	24.369	15.274	5.154	1.00	11.65	H	O
ATOM	1433	N	ALA	H	55	26.740	16.085	6.321	1.00	12.45	H	N
ATOM	1434	CA	ALA	H	55	28.178	15.888	6.507	1.00	12.19	H	C
ATOM	1435	C	ALA	H	55	28.911	15.910	5.166	1.00	12.89	H	C
ATOM	1436	O	ALA	H	55	28.422	15.377	4.169	1.00	12.34	H	O
ATOM	1437	CB	ALA	H	55	28.440	14.565	7.219	1.00	10.54	H	C
ATOM	1438	N	ALA	H	56	30.087	16.528	5.146	1.00	11.36	H	N
ATOM	1439	CA	ALA	H	56	30.880	16.606	3.925	1.00	12.72	H	C
ATOM	1440	C	ALA	H	56	31.315	15.244	3.387	1.00	13.03	H	C
ATOM	1441	O	ALA	H	56	31.283	15.021	2.172	1.00	13.79	H	O
ATOM	1442	CB	ALA	H	56	32.122	17.481	4.156	1.00	12.20	H	C
ATOM	1443	N	HIS	H	57	31.720	14.327	4.266	1.00	12.47	H	N
ATOM	1444	CA	HIS	H	57	32.187	13.025	3.791	1.00	14.60	H	C
ATOM	1445	C	HIS	H	57	31.136	12.203	3.039	1.00	16.39	H	C
ATOM	1446	O	HIS	H	57	31.470	11.252	2.332	1.00	16.35	H	O
ATOM	1447	CB	HIS	H	57	32.798	12.200	4.937	1.00	13.36	H	C

ATOM	1448	CG	HIS	H	57	31.807	11.425	5.749	1.00	11.86	H	C
ATOM	1449	ND1	HIS	H	57	31.362	11.849	6.983	1.00	8.73	H	N
ATOM	1450	CD2	HIS	H	57	31.219	10.222	5.530	1.00	9.58	H	C
ATOM	1451	CE1	HIS	H	57	30.547	10.941	7.491	1.00	9.27	H	C
ATOM	1452	NE2	HIS	H	57	30.443	9.945	6.630	1.00	9.58	H	N
ATOM	1453	N	CYS	H	58	29.869	12.581	3.175	1.00	16.13	H	N
ATOM	1454	CA	CYS	H	58	28.789	11.887	2.485	1.00	16.63	H	C
ATOM	1455	C	CYS	H	58	28.880	12.061	0.967	1.00	15.55	H	C
ATOM	1456	O	CYS	H	58	28.248	11.329	0.208	1.00	14.79	H	O
ATOM	1457	CB	CYS	H	58	27.443	12.426	2.979	1.00	17.08	H	C
ATOM	1458	SG	CYS	H	58	27.023	11.898	4.670	1.00	18.19	H	S
ATOM	1459	N	PHE	H	59	29.675	13.030	0.532	1.00	15.81	H	N
ATOM	1460	CA	PHE	H	59	29.826	13.327	-0.883	1.00	14.61	H	C
ATOM	1461	C	PHE	H	59	31.191	12.959	-1.475	1.00	14.54	H	C
ATOM	1462	O	PHE	H	59	31.504	13.349	-2.602	1.00	13.82	H	O
ATOM	1463	CB	PHE	H	59	29.517	14.816	-1.094	1.00	14.40	H	C
ATOM	1464	CG	PHE	H	59	28.188	15.231	-0.517	1.00	15.03	H	C
ATOM	1465	CD1	PHE	H	59	27.008	14.984	-1.210	1.00	14.65	H	C
ATOM	1466	CD2	PHE	H	59	28.109	15.765	0.770	1.00	14.34	H	C
ATOM	1467	CE1	PHE	H	59	25.768	15.252	-0.629	1.00	15.30	H	C
ATOM	1468	CE2	PHE	H	59	26.875	16.033	1.358	1.00	14.77	H	C
ATOM	1469	CZ	PHE	H	59	25.703	15.774	0.657	1.00	16.63	H	C
ATOM	1470	N	ASP	H	60	31.986	12.195	-0.727	1.00	14.66	H	N
ATOM	1471	CA	ASP	H	60	33.313	11.761	-1.179	1.00	16.60	H	C
ATOM	1472	C	ASP	H	60	33.310	10.997	-2.509	1.00	18.45	H	C
ATOM	1473	O	ASP	H	60	34.172	11.216	-3.358	1.00	17.09	H	O
ATOM	1474	CB	ASP	H	60	33.979	10.872	-0.117	1.00	15.71	H	C
ATOM	1475	CG	ASP	H	60	34.633	11.668	0.998	1.00	15.52	H	C
ATOM	1476	OD1	ASP	H	60	34.520	12.897	1.005	1.00	13.68	H	O
ATOM	1477	OD2	ASP	H	60	35.262	11.049	1.855	1.00	15.21	H	O
ATOM	1478	N	LYS	H	60A	32.357	10.089	-2.687	1.00	21.04	H	N
ATOM	1479	CA	LYS	H	60A	32.303	9.306	-3.918	1.00	23.97	H	C
ATOM	1480	C	LYS	H	60A	31.110	9.568	-4.830	1.00	24.27	H	C
ATOM	1481	O	LYS	H	60A	30.675	8.678	-5.558	1.00	24.87	H	O
ATOM	1482	CB	LYS	H	60A	32.372	7.813	-3.599	1.00	26.20	H	C
ATOM	1483	CG	LYS	H	60A	33.775	7.323	-3.279	1.00	32.13	H	C
ATOM	1484	CD	LYS	H	60A	34.039	7.276	-1.794	1.00	35.71	H	C
ATOM	1485	CE	LYS	H	60A	33.231	6.169	-1.128	1.00	38.10	H	C
ATOM	1486	NZ	LYS	H	60A	33.565	6.052	0.323	1.00	42.45	H	N
ATOM	1487	N	ILE	H	60B	30.583	10.785	-4.796	1.00	25.56	H	N
ATOM	1488	CA	ILE	H	60B	29.454	11.132	-5.642	1.00	25.53	H	C
ATOM	1489	C	ILE	H	60B	29.979	11.394	-7.049	1.00	28.48	H	C
ATOM	1490	O	ILE	H	60B	30.919	12.168	-7.232	1.00	28.70	H	O
ATOM	1491	CB	ILE	H	60B	28.736	12.409	-5.143	1.00	24.23	H	C
ATOM	1492	CG1	ILE	H	60B	28.147	12.180	-3.746	1.00	22.79	H	C
ATOM	1493	CG2	ILE	H	60B	27.647	12.807	-6.132	1.00	24.21	H	C
ATOM	1494	CD1	ILE	H	60B	27.036	11.148	-3.688	1.00	19.86	H	C
ATOM	1495	N	LYS	H	60C	29.378	10.734	-8.034	1.00	29.76	H	N
ATOM	1496	CA	LYS	H	60C	29.764	10.902	-9.430	1.00	31.95	H	C
ATOM	1497	C	LYS	H	60C	28.665	11.565	-10.169	1.00	31.45	H	C
ATOM	1498	O	LYS	H	60C	28.942	12.513	-11.015	1.00	32.26	H	O
ATOM	1499	CB	LYS	H	60C	29.974	9.536	-10.091	1.00	35.12	H	C
ATOM	1500	CG	LYS	H	60C	31.059	8.679	-9.440	1.00	38.59	H	C
ATOM	1501	CD	LYS	H	60C	32.462	9.191	-9.753	1.00	41.77	H	C
ATOM	1502	CE	LYS	H	60C	33.034	8.561	-11.024	1.00	43.81	H	C
ATOM	1503	NZ	LYS	H	60C	32.241	8.847	-12.257	1.00	46.15	H	N

ATOM	1504	N	ASN	H	60D	27.415	11.360	-9.834	1.00	30.75	H	N
ATOM	1505	CA	ASN	H	60D	26.272	12.005	-10.464	1.00	29.53	H	C
ATOM	1506	C	ASN	H	60D	25.675	13.073	-9.549	1.00	28.25	H	C
ATOM	1507	O	ASN	H	60D	24.678	12.833	-8.858	1.00	26.07	H	O
ATOM	1508	CB	ASN	H	60D	25.203	10.963	-10.803	1.00	32.77	H	C
ATOM	1509	CG	ASN	H	60D	25.726	9.853	-11.700	1.00	35.73	H	C
ATOM	1510	OD1	ASN	H	60D	26.355	10.111	-12.727	1.00	37.75	H	O
ATOM	1511	ND2	ASN	H	60D	25.454	8.609	-11.320	1.00	37.39	H	N
ATOM	1512	N	TRP	H	61	26.279	14.256	-9.567	1.00	25.37	H	N
ATOM	1513	CA	TRP	H	61	25.834	15.365	-8.734	1.00	25.31	H	C
ATOM	1514	C	TRP	H	61	24.422	15.863	-9.016	1.00	26.09	H	C
ATOM	1515	O	TRP	H	61	23.849	16.582	-8.203	1.00	25.00	H	O
ATOM	1516	CB	TRP	H	61	26.822	16.532	-8.839	1.00	24.50	H	C
ATOM	1517	CG	TRP	H	61	28.179	16.178	-8.321	1.00	21.92	H	C
ATOM	1518	CD1	TRP	H	61	29.211	15.634	-9.027	1.00	21.98	H	C
ATOM	1519	CD2	TRP	H	61	28.615	16.247	-6.961	1.00	20.82	H	C
ATOM	1520	NE1	TRP	H	61	30.262	15.355	-8.189	1.00	22.70	H	N
ATOM	1521	CE2	TRP	H	61	29.921	15.722	-6.912	1.00	20.71	H	C
ATOM	1522	CE3	TRP	H	61	28.025	16.703	-5.772	1.00	19.10	H	C
ATOM	1523	CZ2	TRP	H	61	30.651	15.634	-5.724	1.00	17.70	H	C
ATOM	1524	CZ3	TRP	H	61	28.749	16.616	-4.593	1.00	17.89	H	C
ATOM	1525	CH2	TRP	H	61	30.050	16.084	-4.579	1.00	17.22	H	C
ATOM	1526	N	ARG	H	62	23.858	15.492	-10.160	1.00	26.23	H	N
ATOM	1527	CA	ARG	H	62	22.503	15.919	-10.494	1.00	28.01	H	C
ATOM	1528	C	ARG	H	62	21.432	14.938	-10.009	1.00	26.66	H	C
ATOM	1529	O	ARG	H	62	20.240	15.216	-10.125	1.00	25.99	H	O
ATOM	1530	CB	ARG	H	62	22.365	16.136	-12.007	1.00	31.33	H	C
ATOM	1531	CG	ARG	H	62	22.965	17.448	-12.509	1.00	36.27	H	C
ATOM	1532	CD	ARG	H	62	22.697	17.657	-13.997	1.00	40.57	H	C
ATOM	1533	NE	ARG	H	62	23.530	16.804	-14.844	1.00	44.43	H	N
ATOM	1534	CZ	ARG	H	62	24.787	17.078	-15.190	1.00	46.30	H	C
ATOM	1535	NH1	ARG	H	62	25.374	18.192	-14.770	1.00	46.47	H	N
ATOM	1536	NH2	ARG	H	62	25.462	16.229	-15.954	1.00	45.81	H	N
ATOM	1537	N	ASN	H	63	21.854	13.802	-9.459	1.00	25.42	H	N
ATOM	1538	CA	ASN	H	63	20.917	12.797	-8.958	1.00	25.01	H	C
ATOM	1539	C	ASN	H	63	20.829	12.745	-7.431	1.00	24.39	H	C
ATOM	1540	O	ASN	H	63	20.573	11.682	-6.860	1.00	24.25	H	O
ATOM	1541	CB	ASN	H	63	21.296	11.404	-9.468	1.00	27.47	H	C
ATOM	1542	CG	ASN	H	63	21.396	11.341	-10.976	1.00	31.32	H	C
ATOM	1543	OD1	ASN	H	63	20.715	12.078	-11.686	1.00	31.92	H	O
ATOM	1544	ND2	ASN	H	63	22.238	10.442	-11.476	1.00	32.46	H	N
ATOM	1545	N	LEU	H	64	21.047	13.875	-6.767	1.00	21.76	H	N
ATOM	1546	CA	LEU	H	64	20.966	13.910	-5.309	1.00	20.28	H	C
ATOM	1547	C	LEU	H	64	19.568	14.341	-4.862	1.00	19.50	H	C
ATOM	1548	O	LEU	H	64	19.071	15.395	-5.268	1.00	18.78	H	O
ATOM	1549	CB	LEU	H	64	22.018	14.855	-4.744	1.00	19.05	H	C
ATOM	1550	CG	LEU	H	64	23.464	14.353	-4.771	1.00	20.72	H	C
ATOM	1551	CD1	LEU	H	64	24.424	15.537	-4.548	1.00	20.72	H	C
ATOM	1552	CD2	LEU	H	64	23.654	13.282	-3.702	1.00	18.65	H	C
ATOM	1553	N	ILE	H	65	18.938	13.520	-4.027	1.00	17.67	H	N
ATOM	1554	CA	ILE	H	65	17.589	13.810	-3.539	1.00	18.01	H	C
ATOM	1555	C	ILE	H	65	17.541	13.931	-2.015	1.00	16.76	H	C
ATOM	1556	O	ILE	H	65	18.200	13.172	-1.303	1.00	14.51	H	O
ATOM	1557	CB	ILE	H	65	16.592	12.692	-3.980	1.00	18.70	H	C
ATOM	1558	CG1	ILE	H	65	16.468	12.671	-5.508	1.00	19.21	H	C
ATOM	1559	CG2	ILE	H	65	15.215	12.918	-3.352	1.00	19.44	H	C

ATOM	1560	CD1	ILE	H	65	15.788	13.897	-6.089	1.00	17.74	H	C
ATOM	1561	N	ALA	H	66	16.774	14.903	-1.527	1.00	15.47	H	N
ATOM	1562	CA	ALA	H	66	16.603	15.111	-0.097	1.00	15.47	H	C
ATOM	1563	C	ALA	H	66	15.125	14.876	0.196	1.00	16.47	H	C
ATOM	1564	O	ALA	H	66	14.254	15.513	-0.405	1.00	16.85	H	O
ATOM	1565	CB	ALA	H	66	16.995	16.531	0.290	1.00	12.74	H	C
ATOM	1566	N	VAL	H	67	14.844	13.954	1.108	1.00	14.86	H	N
ATOM	1567	CA	VAL	H	67	13.469	13.643	1.459	1.00	16.12	H	C
ATOM	1568	C	VAL	H	67	13.169	14.082	2.894	1.00	16.69	H	C
ATOM	1569	O	VAL	H	67	13.895	13.732	3.832	1.00	14.62	H	O
ATOM	1570	CB	VAL	H	67	13.184	12.123	1.323	1.00	17.25	H	C
ATOM	1571	CG1	VAL	H	67	11.695	11.856	1.492	1.00	18.41	H	C
ATOM	1572	CG2	VAL	H	67	13.652	11.616	-0.045	1.00	15.42	H	C
ATOM	1573	N	LEU	H	68	12.111	14.875	3.042	1.00	14.71	H	N
ATOM	1574	CA	LEU	H	68	11.662	15.368	4.341	1.00	14.94	H	C
ATOM	1575	C	LEU	H	68	10.368	14.648	4.744	1.00	14.41	H	C
ATOM	1576	O	LEU	H	68	9.639	14.144	3.888	1.00	15.50	H	O
ATOM	1577	CB	LEU	H	68	11.409	16.881	4.282	1.00	11.00	H	C
ATOM	1578	CG	LEU	H	68	12.589	17.836	4.542	1.00	14.28	H	C
ATOM	1579	CD1	LEU	H	68	13.204	17.495	5.901	1.00	14.52	H	C
ATOM	1580	CD2	LEU	H	68	13.645	17.729	3.445	1.00	12.56	H	C
ATOM	1581	N	GLY	H	69	10.098	14.593	6.047	1.00	13.97	H	N
ATOM	1582	CA	GLY	H	69	8.890	13.951	6.547	1.00	13.77	H	C
ATOM	1583	C	GLY	H	69	8.913	12.438	6.465	1.00	17.11	H	C
ATOM	1584	O	GLY	H	69	7.886	11.774	6.637	1.00	17.76	H	O
ATOM	1585	N	GLU	H	70	10.096	11.889	6.211	1.00	16.90	H	N
ATOM	1586	CA	GLU	H	70	10.275	10.454	6.101	1.00	16.57	H	C
ATOM	1587	C	GLU	H	70	10.245	9.800	7.491	1.00	16.50	H	C
ATOM	1588	O	GLU	H	70	10.567	10.437	8.494	1.00	15.98	H	O
ATOM	1589	CB	GLU	H	70	11.602	10.174	5.387	1.00	19.03	H	C
ATOM	1590	CG	GLU	H	70	11.865	8.726	5.080	1.00	22.67	H	C
ATOM	1591	CD	GLU	H	70	10.684	8.066	4.398	1.00	25.35	H	C
ATOM	1592	OE1	GLU	H	70	10.563	8.141	3.189	1.00	24.42	H	O
ATOM	1593	OE2	GLU	H	70	9.892	7.495	5.098	1.00	23.25	H	O
ATOM	1594	N	HIS	H	71	9.813	8.544	7.546	1.00	12.74	H	N
ATOM	1595	CA	HIS	H	71	9.761	7.801	8.799	1.00	13.45	H	C
ATOM	1596	C	HIS	H	71	10.080	6.321	8.586	1.00	12.69	H	C
ATOM	1597	O	HIS	H	71	11.080	5.815	9.091	1.00	11.97	H	O
ATOM	1598	CB	HIS	H	71	8.380	7.919	9.455	1.00	12.65	H	C
ATOM	1599	CG	HIS	H	71	8.219	7.045	10.659	1.00	14.72	H	C
ATOM	1600	ND1	HIS	H	71	8.933	7.245	11.821	1.00	15.86	H	N
ATOM	1601	CD2	HIS	H	71	7.488	5.922	10.857	1.00	15.60	H	C
ATOM	1602	CE1	HIS	H	71	8.652	6.281	12.680	1.00	15.50	H	C
ATOM	1603	NE2	HIS	H	71	7.778	5.465	12.119	1.00	16.25	H	N
ATOM	1604	N	ASP	H	72	9.214	5.642	7.836	1.00	12.78	H	N
ATOM	1605	CA	ASP	H	72	9.340	4.213	7.543	1.00	14.80	H	C
ATOM	1606	C	ASP	H	72	9.726	4.058	6.078	1.00	14.88	H	C
ATOM	1607	O	ASP	H	72	8.931	4.350	5.200	1.00	14.21	H	O
ATOM	1608	CB	ASP	H	72	7.988	3.539	7.798	1.00	17.28	H	C
ATOM	1609	CG	ASP	H	72	8.012	2.046	7.555	1.00	20.88	H	C
ATOM	1610	OD1	ASP	H	72	8.887	1.559	6.837	1.00	18.95	H	O
ATOM	1611	OD2	ASP	H	72	7.134	1.377	8.082	1.00	22.75	H	O
ATOM	1612	N	LEU	H	73	10.936	3.587	5.805	1.00	16.56	H	N
ATOM	1613	CA	LEU	H	73	11.385	3.443	4.423	1.00	16.35	H	C
ATOM	1614	C	LEU	H	73	10.650	2.377	3.596	1.00	18.34	H	C
ATOM	1615	O	LEU	H	73	10.858	2.282	2.385	1.00	19.52	H	O

ATOM	1616	CB	LEU	H	73	12.895	3.171	4.397	1.00	16.77	H	C
ATOM	1617	CG	LEU	H	73	13.769	4.110	5.247	1.00	17.81	H	C
ATOM	1618	CD1	LEU	H	73	15.230	3.720	5.100	1.00	15.70	H	C
ATOM	1619	CD2	LEU	H	73	13.555	5.549	4.823	1.00	16.14	H	C
ATOM	1620	N	SER	H	74	9.790	1.590	4.234	1.00	19.10	H	N
ATOM	1621	CA	SER	H	74	9.043	0.548	3.531	1.00	21.62	H	C
ATOM	1622	C	SER	H	74	7.575	0.880	3.242	1.00	23.33	H	C
ATOM	1623	O	SER	H	74	6.867	0.078	2.625	1.00	22.33	H	O
ATOM	1624	CB	SER	H	74	9.114	-0.769	4.308	1.00	20.45	H	C
ATOM	1625	OG	SER	H	74	8.439	-0.675	5.547	1.00	22.87	H	O
ATOM	1626	N	GLU	H	75	7.117	2.053	3.677	1.00	22.57	H	N
ATOM	1627	CA	GLU	H	75	5.732	2.466	3.449	1.00	24.78	H	C
ATOM	1628	C	GLU	H	75	5.688	3.934	3.040	1.00	25.10	H	C
ATOM	1629	O	GLU	H	75	6.318	4.749	3.678	1.00	25.82	H	O
ATOM	1630	CB	GLU	H	75	4.911	2.301	4.730	1.00	26.53	H	C
ATOM	1631	CG	GLU	H	75	4.714	0.873	5.205	1.00	31.89	H	C
ATOM	1632	CD	GLU	H	75	3.839	0.065	4.270	1.00	33.67	H	C
ATOM	1633	OE1	GLU	H	75	2.831	0.603	3.814	1.00	35.97	H	O
ATOM	1634	OE2	GLU	H	75	4.162	-1.102	4.013	1.00	36.04	H	O
ATOM	1635	N	HIS	H	76	4.934	4.275	2.000	1.00	24.98	H	N
ATOM	1636	CA	HIS	H	76	4.830	5.668	1.558	1.00	24.23	H	C
ATOM	1637	C	HIS	H	76	3.569	6.338	2.106	1.00	23.39	H	C
ATOM	1638	O	HIS	H	76	2.514	5.706	2.166	1.00	23.35	H	O
ATOM	1639	CB	HIS	H	76	4.760	5.749	0.026	1.00	25.80	H	C
ATOM	1640	CG	HIS	H	76	6.056	5.469	-0.671	1.00	29.25	H	C
ATOM	1641	ND1	HIS	H	76	7.159	6.288	-0.554	1.00	28.58	H	N
ATOM	1642	CD2	HIS	H	76	6.408	4.488	-1.538	1.00	28.86	H	C
ATOM	1643	CE1	HIS	H	76	8.132	5.827	-1.321	1.00	29.52	H	C
ATOM	1644	NE2	HIS	H	76	7.701	4.736	-1.929	1.00	28.15	H	N
ATOM	1645	N	ASP	H	77	3.677	7.607	2.510	1.00	20.79	H	N
ATOM	1646	CA	ASP	H	77	2.509	8.359	2.973	1.00	19.38	H	C
ATOM	1647	C	ASP	H	77	2.621	9.817	2.533	1.00	18.66	H	C
ATOM	1648	O	ASP	H	77	3.651	10.230	2.004	1.00	21.60	H	O
ATOM	1649	CB	ASP	H	77	2.299	8.257	4.499	1.00	18.12	H	C
ATOM	1650	CG	ASP	H	77	3.384	8.946	5.308	1.00	19.27	H	C
ATOM	1651	OD1	ASP	H	77	3.954	9.946	4.848	1.00	19.03	H	O
ATOM	1652	OD2	ASP	H	77	3.635	8.490	6.418	1.00	17.06	H	O
ATOM	1653	N	GLY	H	78	1.566	10.592	2.755	1.00	18.19	H	N
ATOM	1654	CA	GLY	H	78	1.545	11.980	2.326	1.00	18.10	H	C
ATOM	1655	C	GLY	H	78	2.371	13.025	3.054	1.00	18.55	H	C
ATOM	1656	O	GLY	H	78	2.352	14.197	2.675	1.00	16.08	H	O
ATOM	1657	N	ASP	H	79	3.095	12.625	4.091	1.00	19.01	H	N
ATOM	1658	CA	ASP	H	79	3.910	13.580	4.827	1.00	18.79	H	C
ATOM	1659	C	ASP	H	79	5.297	13.730	4.227	1.00	18.30	H	C
ATOM	1660	O	ASP	H	79	6.014	14.676	4.543	1.00	18.65	H	O
ATOM	1661	CB	ASP	H	79	4.034	13.164	6.295	1.00	19.58	H	C
ATOM	1662	CG	ASP	H	79	2.696	13.111	6.996	1.00	21.14	H	C
ATOM	1663	OD1	ASP	H	79	1.909	14.047	6.832	1.00	22.87	H	O
ATOM	1664	OD2	ASP	H	79	2.450	12.148	7.704	1.00	20.28	H	O
ATOM	1665	N	GLU	H	80	5.685	12.799	3.364	1.00	19.12	H	N
ATOM	1666	CA	GLU	H	80	7.003	12.873	2.758	1.00	20.29	H	C
ATOM	1667	C	GLU	H	80	7.062	13.811	1.563	1.00	19.63	H	C
ATOM	1668	O	GLU	H	80	6.185	13.815	0.699	1.00	19.10	H	O
ATOM	1669	CB	GLU	H	80	7.491	11.472	2.380	1.00	22.03	H	C
ATOM	1670	CG	GLU	H	80	6.528	10.659	1.571	1.00	29.30	H	C
ATOM	1671	CD	GLU	H	80	6.895	9.188	1.567	1.00	29.90	H	C

ATOM	1672	OE1	GLU	H	80	6.763	8.547	2.597	1.00	27.84	H	O
ATOM	1673	OE2	GLU	H	80	7.315	8.707	0.544	1.00	32.19	H	O
ATOM	1674	N	GLN	H	81	8.110	14.625	1.541	1.00	18.82	H	N
ATOM	1675	CA	GLN	H	81	8.324	15.592	0.482	1.00	17.15	H	C
ATOM	1676	C	GLN	H	81	9.723	15.373	-0.065	1.00	18.57	H	C
ATOM	1677	O	GLN	H	81	10.689	15.277	0.691	1.00	18.79	H	O
ATOM	1678	CB	GLN	H	81	8.202	17.004	1.037	1.00	16.07	H	C
ATOM	1679	CG	GLN	H	81	6.873	17.277	1.709	1.00	15.69	H	C
ATOM	1680	CD	GLN	H	81	6.792	18.684	2.237	1.00	13.45	H	C
ATOM	1681	OE1	GLN	H	81	6.982	19.630	1.493	1.00	12.22	H	O
ATOM	1682	NE2	GLN	H	81	6.516	18.828	3.530	1.00	12.50	H	N
ATOM	1683	N	SER	H	82	9.829	15.313	-1.384	1.00	17.31	H	N
ATOM	1684	CA	SER	H	82	11.105	15.072	-2.029	1.00	18.12	H	C
ATOM	1685	C	SER	H	82	11.576	16.299	-2.799	1.00	17.87	H	C
ATOM	1686	O	SER	H	82	10.778	16.996	-3.428	1.00	17.54	H	O
ATOM	1687	CB	SER	H	82	10.965	13.867	-2.960	1.00	16.29	H	C
ATOM	1688	OG	SER	H	82	12.222	13.446	-3.436	1.00	28.10	H	O
ATOM	1689	N	ARG	H	83	12.878	16.563	-2.750	1.00	18.40	H	N
ATOM	1690	CA	ARG	H	83	13.447	17.717	-3.443	1.00	18.45	H	C
ATOM	1691	C	ARG	H	83	14.830	17.401	-3.998	1.00	20.13	H	C
ATOM	1692	O	ARG	H	83	15.629	16.715	-3.354	1.00	21.06	H	O
ATOM	1693	CB	ARG	H	83	13.572	18.906	-2.486	1.00	18.69	H	C
ATOM	1694	CG	ARG	H	83	12.253	19.439	-1.927	1.00	19.20	H	C
ATOM	1695	CD	ARG	H	83	11.544	20.319	-2.947	1.00	17.18	H	C
ATOM	1696	NE	ARG	H	83	10.393	21.010	-2.378	1.00	14.55	H	N
ATOM	1697	CZ	ARG	H	83	9.214	20.444	-2.131	1.00	16.58	H	C
ATOM	1698	NH1	ARG	H	83	9.004	19.159	-2.401	1.00	13.28	H	N
ATOM	1699	NH2	ARG	H	83	8.241	21.170	-1.603	1.00	16.69	H	N
ATOM	1700	N	ARG	H	84	15.116	17.902	-5.194	1.00	19.27	H	N
ATOM	1701	CA	ARG	H	84	16.426	17.697	-5.788	1.00	20.61	H	C
ATOM	1702	C	ARG	H	84	17.392	18.641	-5.075	1.00	18.87	H	C
ATOM	1703	O	ARG	H	84	17.015	19.746	-4.689	1.00	16.00	H	O
ATOM	1704	CB	ARG	H	84	16.414	18.037	-7.283	1.00	23.54	H	C
ATOM	1705	CG	ARG	H	84	15.483	17.186	-8.127	1.00	29.19	H	C
ATOM	1706	CD	ARG	H	84	15.845	17.288	-9.604	1.00	34.52	H	C
ATOM	1707	NE	ARG	H	84	14.872	16.600	-10.451	1.00	40.99	H	N
ATOM	1708	CZ	ARG	H	84	15.065	16.298	-11.733	1.00	44.71	H	C
ATOM	1709	NH1	ARG	H	84	16.206	16.614	-12.337	1.00	46.58	H	N
ATOM	1710	NH2	ARG	H	84	14.110	15.682	-12.417	1.00	46.99	H	N
ATOM	1711	N	VAL	H	85	18.629	18.203	-4.888	1.00	17.74	H	N
ATOM	1712	CA	VAL	H	85	19.622	19.049	-4.243	1.00	16.85	H	C
ATOM	1713	C	VAL	H	85	20.229	19.920	-5.341	1.00	17.99	H	C
ATOM	1714	O	VAL	H	85	20.877	19.416	-6.259	1.00	17.19	H	O
ATOM	1715	CB	VAL	H	85	20.732	18.207	-3.557	1.00	16.36	H	C
ATOM	1716	CG1	VAL	H	85	21.763	19.123	-2.907	1.00	14.96	H	C
ATOM	1717	CG2	VAL	H	85	20.117	17.289	-2.507	1.00	13.28	H	C
ATOM	1718	N	ALA	H	86	19.992	21.227	-5.251	1.00	18.63	H	N
ATOM	1719	CA	ALA	H	86	20.504	22.181	-6.231	1.00	18.54	H	C
ATOM	1720	C	ALA	H	86	21.974	22.513	-6.000	1.00	19.52	H	C
ATOM	1721	O	ALA	H	86	22.692	22.847	-6.942	1.00	20.09	H	O
ATOM	1722	CB	ALA	H	86	19.671	23.471	-6.193	1.00	16.39	H	C
ATOM	1723	N	GLN	H	87	22.424	22.426	-4.752	1.00	18.48	H	N
ATOM	1724	CA	GLN	H	87	23.812	22.739	-4.443	1.00	19.14	H	C
ATOM	1725	C	GLN	H	87	24.330	22.107	-3.149	1.00	17.00	H	C
ATOM	1726	O	GLN	H	87	23.620	22.030	-2.149	1.00	17.11	H	O
ATOM	1727	CB	GLN	H	87	23.986	24.259	-4.376	1.00	20.74	H	C

ATOM	1728	CG	GLN	H	87	25.425	24.729	-4.330	1.00	23.25	H	C
ATOM	1729	CD	GLN	H	87	25.587	26.134	-4.886	1.00	28.67	H	C
ATOM	1730	OE1	GLN	H	87	25.068	27.099	-4.328	1.00	31.99	H	O
ATOM	1731	NE2	GLN	H	87	26.305	26.250	-5.999	1.00	30.93	H	N
ATOM	1732	N	VAL	H	88	25.574	21.645	-3.196	1.00	14.74	H	N
ATOM	1733	CA	VAL	H	88	26.239	21.047	-2.047	1.00	14.64	H	C
ATOM	1734	C	VAL	H	88	27.465	21.920	-1.772	1.00	15.48	H	C
ATOM	1735	O	VAL	H	88	28.404	21.946	-2.562	1.00	17.00	H	O
ATOM	1736	CB	VAL	H	88	26.705	19.606	-2.347	1.00	14.89	H	C
ATOM	1737	CG1	VAL	H	88	27.474	19.046	-1.155	1.00	14.11	H	C
ATOM	1738	CG2	VAL	H	88	25.506	18.726	-2.680	1.00	14.41	H	C
ATOM	1739	N	ILE	H	89	27.443	22.646	-0.662	1.00	15.46	H	N
ATOM	1740	CA	ILE	H	89	28.545	23.523	-0.300	1.00	14.42	H	C
ATOM	1741	C	ILE	H	89	29.390	22.884	0.794	1.00	15.81	H	C
ATOM	1742	O	ILE	H	89	28.897	22.549	1.876	1.00	16.16	H	O
ATOM	1743	CB	ILE	H	89	28.030	24.884	0.190	1.00	13.77	H	C
ATOM	1744	CG1	ILE	H	89	27.072	25.485	-0.847	1.00	14.85	H	C
ATOM	1745	CG2	ILE	H	89	29.209	25.829	0.413	1.00	14.01	H	C
ATOM	1746	CD1	ILE	H	89	26.360	26.755	-0.384	1.00	13.34	H	C
ATOM	1747	N	ILE	H	90	30.674	22.724	0.500	1.00	15.61	H	N
ATOM	1748	CA	ILE	H	90	31.619	22.110	1.421	1.00	15.21	H	C
ATOM	1749	C	ILE	H	90	32.777	23.066	1.691	1.00	15.60	H	C
ATOM	1750	O	ILE	H	90	33.197	23.804	0.802	1.00	16.74	H	O
ATOM	1751	CB	ILE	H	90	32.151	20.789	0.802	1.00	15.99	H	C
ATOM	1752	CG1	ILE	H	90	31.018	19.759	0.760	1.00	15.68	H	C
ATOM	1753	CG2	ILE	H	90	33.339	20.254	1.590	1.00	17.02	H	C
ATOM	1754	CD1	ILE	H	90	31.365	18.486	0.005	1.00	19.51	H	C
ATOM	1755	N	PRO	H	91	33.297	23.081	2.931	1.00	16.87	H	N
ATOM	1756	CA	PRO	H	91	34.415	23.971	3.259	1.00	14.80	H	C
ATOM	1757	C	PRO	H	91	35.627	23.649	2.384	1.00	15.40	H	C
ATOM	1758	O	PRO	H	91	35.917	22.480	2.120	1.00	12.85	H	O
ATOM	1759	CB	PRO	H	91	34.692	23.657	4.728	1.00	15.20	H	C
ATOM	1760	CG	PRO	H	91	33.360	23.185	5.241	1.00	16.50	H	C
ATOM	1761	CD	PRO	H	91	32.867	22.319	4.118	1.00	15.23	H	C
ATOM	1762	N	SER	H	92	36.336	24.681	1.939	1.00	14.94	H	N
ATOM	1763	CA	SER	H	92	37.521	24.471	1.114	1.00	15.06	H	C
ATOM	1764	C	SER	H	92	38.598	23.704	1.888	1.00	14.20	H	C
ATOM	1765	O	SER	H	92	39.489	23.117	1.289	1.00	15.42	H	O
ATOM	1766	CB	SER	H	92	38.084	25.813	0.643	1.00	14.89	H	C
ATOM	1767	OG	SER	H	92	37.144	26.502	-0.166	1.00	15.02	H	O
ATOM	1768	N	THR	H	93	38.497	23.701	3.214	1.00	12.98	H	N
ATOM	1769	CA	THR	H	93	39.461	23.020	4.072	1.00	13.34	H	C
ATOM	1770	C	THR	H	93	39.182	21.531	4.309	1.00	14.82	H	C
ATOM	1771	O	THR	H	93	39.994	20.840	4.916	1.00	15.40	H	O
ATOM	1772	CB	THR	H	93	39.556	23.716	5.448	1.00	14.87	H	C
ATOM	1773	OG1	THR	H	93	38.249	23.788	6.033	1.00	11.15	H	O
ATOM	1774	CG2	THR	H	93	40.133	25.140	5.302	1.00	11.43	H	C
ATOM	1775	N	TYR	H	94	38.040	21.033	3.847	1.00	14.91	H	N
ATOM	1776	CA	TYR	H	94	37.724	19.618	4.024	1.00	14.16	H	C
ATOM	1777	C	TYR	H	94	38.482	18.783	2.989	1.00	14.17	H	C
ATOM	1778	O	TYR	H	94	38.558	19.151	1.822	1.00	14.26	H	O
ATOM	1779	CB	TYR	H	94	36.220	19.366	3.862	1.00	12.83	H	C
ATOM	1780	CG	TYR	H	94	35.874	17.888	3.785	1.00	11.02	H	C
ATOM	1781	CD1	TYR	H	94	35.851	17.101	4.931	1.00	9.72	H	C
ATOM	1782	CD2	TYR	H	94	35.656	17.264	2.552	1.00	11.67	H	C
ATOM	1783	CE1	TYR	H	94	35.629	15.728	4.858	1.00	8.62	H	C

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ATOM   1784  CE2 TYR H  94      35.433  15.888   2.467  1.00  8.29      H    C
ATOM   1785  CZ  TYR H  94      35.424  15.130   3.631  1.00  9.43      H    C
ATOM   1786  OH  TYR H  94      35.222  13.773   3.574  1.00 11.83      H    O
ATOM   1787  N   VAL H  95      39.048  17.664   3.423  1.00 13.98      H    N
ATOM   1788  CA  VAL H  95      39.771  16.775   2.519  1.00 13.14      H    C
ATOM   1789  C   VAL H  95      39.041  15.431   2.436  1.00 12.82      H    C
ATOM   1790  O   VAL H  95      38.845  14.761   3.444  1.00 13.46      H    O
ATOM   1791  CB  VAL H  95      41.219  16.517   3.006  1.00 11.88      H    C
ATOM   1792  CG1 VAL H  95      41.922  15.540   2.062  1.00 10.92      H    C
ATOM   1793  CG2 VAL H  95      41.992  17.826   3.065  1.00 11.07      H    C
ATOM   1794  N   PRO H  96      38.624  15.025   1.229  1.00 12.92      H    N
ATOM   1795  CA  PRO H  96      37.922  13.749   1.062  1.00 11.72      H    C
ATOM   1796  C   PRO H  96      38.730  12.604   1.675  1.00 13.96      H    C
ATOM   1797  O   PRO H  96      39.957  12.548   1.525  1.00 15.05      H    O
ATOM   1798  CB  PRO H  96      37.809  13.620  -0.453  1.00  9.89      H    C
ATOM   1799  CG  PRO H  96      37.671  15.048  -0.885  1.00 12.78      H    C
ATOM   1800  CD  PRO H  96      38.742  15.730  -0.060  1.00 12.59      H    C
ATOM   1801  N   GLY H  97      38.038  11.697   2.354  1.00 12.86      H    N
ATOM   1802  CA  GLY H  97      38.698  10.574   2.986  1.00 13.45      H    C
ATOM   1803  C   GLY H  97      39.107  10.871   4.418  1.00 15.29      H    C
ATOM   1804  O   GLY H  97      39.539   9.967   5.131  1.00 15.13      H    O
ATOM   1805  N   THR H  98      38.972  12.127   4.846  1.00 15.09      H    N
ATOM   1806  CA  THR H  98      39.356  12.509   6.202  1.00 15.44      H    C
ATOM   1807  C   THR H  98      38.173  12.924   7.082  1.00 15.39      H    C
ATOM   1808  O   THR H  98      37.014  12.798   6.679  1.00 15.40      H    O
ATOM   1809  CB  THR H  98      40.417  13.631   6.185  1.00 16.79      H    C
ATOM   1810  OG1 THR H  98      39.864  14.813   5.605  1.00 16.68      H    O
ATOM   1811  CG2 THR H  98      41.631  13.193   5.375  1.00 17.03      H    C
ATOM   1812  N   THR H  99      38.469  13.433   8.275  1.00 14.02      H    N
ATOM   1813  CA  THR H  99      37.429  13.783   9.236  1.00 14.07      H    C
ATOM   1814  C   THR H  99      37.206  15.251   9.633  1.00 14.00      H    C
ATOM   1815  O   THR H  99      36.111  15.605  10.086  1.00 11.58      H    O
ATOM   1816  CB  THR H  99      37.643  12.963  10.532  1.00 16.74      H    C
ATOM   1817  OG1 THR H  99      38.973  13.187  11.022  1.00 17.73      H    O
ATOM   1818  CG2 THR H  99      37.468  11.465  10.265  1.00 15.58      H    C
ATOM   1819  N   ASN H 100      38.219  16.102   9.473  1.00 11.56      H    N
ATOM   1820  CA  ASN H 100      38.097  17.512   9.859  1.00 11.57      H    C
ATOM   1821  C   ASN H 100      37.189  18.315   8.927  1.00  9.66      H    C
ATOM   1822  O   ASN H 100      37.165  18.086   7.719  1.00 11.07      H    O
ATOM   1823  CB  ASN H 100      39.485  18.181   9.911  1.00  9.81      H    C
ATOM   1824  CG  ASN H 100      39.576  19.288  10.966  1.00 12.61      H    C
ATOM   1825  OD1 ASN H 100      40.498  20.112  10.939  1.00 15.96      H    O
ATOM   1826  ND2 ASN H 100      38.633  19.300  11.908  1.00  7.34      H    N
ATOM   1827  N   HIS H 101      36.455  19.264   9.500  1.00  9.02      H    N
ATOM   1828  CA  HIS H 101      35.552  20.124   8.738  1.00 10.03      H    C
ATOM   1829  C   HIS H 101      34.503  19.292   8.017  1.00  9.38      H    C
ATOM   1830  O   HIS H 101      34.188  19.544   6.857  1.00  8.47      H    O
ATOM   1831  CB  HIS H 101      36.347  20.953   7.724  1.00 11.39      H    C
ATOM   1832  CG  HIS H 101      37.353  21.868   8.352  1.00 16.40      H    C
ATOM   1833  ND1 HIS H 101      36.997  22.895   9.200  1.00 18.05      H    N
ATOM   1834  CD2 HIS H 101      38.705  21.882   8.293  1.00 17.22      H    C
ATOM   1835  CE1 HIS H 101      38.086  23.501   9.639  1.00 18.13      H    C
ATOM   1836  NE2 HIS H 101      39.137  22.906   9.103  1.00 17.47      H    N
ATOM   1837  N   ASP H 102      33.958  18.305   8.720  1.00  8.97      H    N
ATOM   1838  CA  ASP H 102      32.967  17.407   8.148  1.00 10.95      H    C
ATOM   1839  C   ASP H 102      31.567  18.022   8.153  1.00 10.99      H    C
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ATOM	1840	O	ASP	H	102	30.699	17.621	8.935	1.00	10.41	H O
ATOM	1841	CB	ASP	H	102	32.971	16.092	8.928	1.00	9.16	H C
ATOM	1842	CG	ASP	H	102	32.360	14.959	8.147	1.00	12.94	H C
ATOM	1843	OD1	ASP	H	102	32.039	15.173	6.976	1.00	11.04	H O
ATOM	1844	OD2	ASP	H	102	32.216	13.870	8.703	1.00	12.25	H O
ATOM	1845	N	ILE	H	103	31.351	18.993	7.271	1.00	10.37	H N
ATOM	1846	CA	ILE	H	103	30.061	19.672	7.192	1.00	8.57	H C
ATOM	1847	C	ILE	H	103	29.730	20.071	5.760	1.00	9.30	H C
ATOM	1848	O	ILE	H	103	30.621	20.374	4.962	1.00	8.92	H O
ATOM	1849	CB	ILE	H	103	30.058	20.941	8.084	1.00	10.09	H C
ATOM	1850	CG1	ILE	H	103	28.677	21.607	8.072	1.00	7.85	H C
ATOM	1851	CG2	ILE	H	103	31.120	21.923	7.591	1.00	9.32	H C
ATOM	1852	CD1	ILE	H	103	28.502	22.665	9.152	1.00	11.15	H C
ATOM	1853	N	ALA	H	104	28.442	20.055	5.437	1.00	9.70	H N
ATOM	1854	CA	ALA	H	104	27.970	20.445	4.114	1.00	10.78	H C
ATOM	1855	C	ALA	H	104	26.639	21.173	4.248	1.00	12.66	H C
ATOM	1856	O	ALA	H	104	25.789	20.804	5.063	1.00	11.86	H O
ATOM	1857	CB	ALA	H	104	27.807	19.217	3.216	1.00	7.13	H C
ATOM	1858	N	LEU	H	105	26.482	22.226	3.454	1.00	14.56	H N
ATOM	1859	CA	LEU	H	105	25.258	23.016	3.426	1.00	12.91	H C
ATOM	1860	C	LEU	H	105	24.640	22.753	2.057	1.00	12.76	H C
ATOM	1861	O	LEU	H	105	25.243	23.065	1.029	1.00	12.63	H O
ATOM	1862	CB	LEU	H	105	25.580	24.504	3.576	1.00	12.35	H C
ATOM	1863	CG	LEU	H	105	24.389	25.466	3.494	1.00	12.09	H C
ATOM	1864	CD1	LEU	H	105	23.413	25.197	4.641	1.00	9.27	H C
ATOM	1865	CD2	LEU	H	105	24.903	26.892	3.560	1.00	9.24	H C
ATOM	1866	N	LEU	H	106	23.445	22.172	2.046	1.00	12.35	H N
ATOM	1867	CA	LEU	H	106	22.758	21.837	0.803	1.00	11.43	H C
ATOM	1868	C	LEU	H	106	21.564	22.748	0.515	1.00	12.98	H C
ATOM	1869	O	LEU	H	106	20.726	22.978	1.384	1.00	12.54	H O
ATOM	1870	CB	LEU	H	106	22.285	20.380	0.859	1.00	12.53	H C
ATOM	1871	CG	LEU	H	106	23.263	19.202	0.659	1.00	14.01	H C
ATOM	1872	CD1	LEU	H	106	24.503	19.322	1.539	1.00	12.26	H C
ATOM	1873	CD2	LEU	H	106	22.519	17.906	0.983	1.00	12.82	H C
ATOM	1874	N	ARG	H	107	21.492	23.278	-0.703	1.00	14.02	H N
ATOM	1875	CA	ARG	H	107	20.370	24.128	-1.077	1.00	16.64	H C
ATOM	1876	C	ARG	H	107	19.397	23.266	-1.873	1.00	16.72	H C
ATOM	1877	O	ARG	H	107	19.791	22.591	-2.819	1.00	18.56	H O
ATOM	1878	CB	ARG	H	107	20.822	25.313	-1.942	1.00	18.34	H C
ATOM	1879	CG	ARG	H	107	19.754	26.410	-2.081	1.00	20.80	H C
ATOM	1880	CD	ARG	H	107	19.992	27.301	-3.302	1.00	26.37	H C
ATOM	1881	NE	ARG	H	107	21.234	28.069	-3.224	1.00	29.38	H N
ATOM	1882	CZ	ARG	H	107	21.321	29.337	-2.827	1.00	30.69	H C
ATOM	1883	NH1	ARG	H	107	20.233	30.007	-2.463	1.00	31.39	H N
ATOM	1884	NH2	ARG	H	107	22.503	29.940	-2.798	1.00	29.68	H N
ATOM	1885	N	LEU	H	108	18.131	23.280	-1.480	1.00	16.62	H N
ATOM	1886	CA	LEU	H	108	17.114	22.500	-2.170	1.00	17.28	H C
ATOM	1887	C	LEU	H	108	16.608	23.281	-3.385	1.00	18.87	H C
ATOM	1888	O	LEU	H	108	16.532	24.510	-3.349	1.00	18.26	H O
ATOM	1889	CB	LEU	H	108	15.962	22.188	-1.208	1.00	15.65	H C
ATOM	1890	CG	LEU	H	108	16.352	21.391	0.050	1.00	14.18	H C
ATOM	1891	CD1	LEU	H	108	15.134	21.191	0.953	1.00	10.37	H C
ATOM	1892	CD2	LEU	H	108	16.942	20.041	-0.361	1.00	11.86	H C
ATOM	1893	N	HIS	H	109	16.273	22.568	-4.457	1.00	20.64	H N
ATOM	1894	CA	HIS	H	109	15.790	23.205	-5.683	1.00	22.07	H C
ATOM	1895	C	HIS	H	109	14.546	24.054	-5.430	1.00	21.71	H C

ATOM	1896	O	HIS	H	109	14.399	25.139	-5.986	1.00	21.72	H O
ATOM	1897	CB	HIS	H	109	15.467	22.155	-6.746	1.00	24.90	H C
ATOM	1898	CG	HIS	H	109	15.022	22.742	-8.048	1.00	28.69	H C
ATOM	1899	ND1	HIS	H	109	13.921	22.279	-8.738	1.00	31.80	H N
ATOM	1900	CD2	HIS	H	109	15.525	23.762	-8.784	1.00	30.89	H C
ATOM	1901	CE1	HIS	H	109	13.766	22.989	-9.842	1.00	31.18	H C
ATOM	1902	NE2	HIS	H	109	14.726	23.895	-9.894	1.00	30.63	H N
ATOM	1903	N	GLN	H	110	13.647	23.541	-4.603	1.00	19.28	H N
ATOM	1904	CA	GLN	H	110	12.430	24.252	-4.258	1.00	21.37	H C
ATOM	1905	C	GLN	H	110	12.219	24.059	-2.766	1.00	19.91	H C
ATOM	1906	O	GLN	H	110	12.566	23.014	-2.210	1.00	19.14	H O
ATOM	1907	CB	GLN	H	110	11.230	23.689	-5.030	1.00	24.70	H C
ATOM	1908	CG	GLN	H	110	11.340	23.814	-6.551	1.00	33.11	H C
ATOM	1909	CD	GLN	H	110	11.188	25.245	-7.075	1.00	37.50	H C
ATOM	1910	OE1	GLN	H	110	11.434	25.505	-8.254	1.00	42.27	H O
ATOM	1911	NE2	GLN	H	110	10.772	26.168	-6.212	1.00	40.37	H N
ATOM	1912	N	PRO	H	111	11.643	25.062	-2.096	1.00	17.61	H N
ATOM	1913	CA	PRO	H	111	11.406	24.959	-0.657	1.00	18.39	H C
ATOM	1914	C	PRO	H	111	10.409	23.869	-0.306	1.00	18.13	H C
ATOM	1915	O	PRO	H	111	9.472	23.615	-1.056	1.00	18.29	H O
ATOM	1916	CB	PRO	H	111	10.882	26.348	-0.299	1.00	18.48	H C
ATOM	1917	CG	PRO	H	111	10.127	26.733	-1.540	1.00	17.21	H C
ATOM	1918	CD	PRO	H	111	11.091	26.319	-2.632	1.00	15.77	H C
ATOM	1919	N	VAL	H	112	10.624	23.215	0.831	1.00	17.13	H N
ATOM	1920	CA	VAL	H	112	9.700	22.189	1.286	1.00	17.69	H C
ATOM	1921	C	VAL	H	112	8.573	22.915	2.013	1.00	16.47	H C
ATOM	1922	O	VAL	H	112	8.708	24.088	2.364	1.00	15.80	H O
ATOM	1923	CB	VAL	H	112	10.371	21.195	2.261	1.00	17.46	H C
ATOM	1924	CG1	VAL	H	112	11.412	20.374	1.526	1.00	19.26	H C
ATOM	1925	CG2	VAL	H	112	10.996	21.945	3.419	1.00	15.83	H C
ATOM	1926	N	VAL	H	113	7.463	22.222	2.228	1.00	15.47	H N
ATOM	1927	CA	VAL	H	113	6.316	22.806	2.912	1.00	13.75	H C
ATOM	1928	C	VAL	H	113	6.395	22.459	4.394	1.00	14.36	H C
ATOM	1929	O	VAL	H	113	6.542	21.290	4.759	1.00	12.82	H O
ATOM	1930	CB	VAL	H	113	4.983	22.247	2.353	1.00	13.88	H C
ATOM	1931	CG1	VAL	H	113	3.808	22.974	2.993	1.00	10.56	H C
ATOM	1932	CG2	VAL	H	113	4.951	22.381	0.821	1.00	12.19	H C
ATOM	1933	N	LEU	H	114	6.305	23.467	5.253	1.00	13.94	H N
ATOM	1934	CA	LEU	H	114	6.363	23.199	6.679	1.00	15.06	H C
ATOM	1935	C	LEU	H	114	5.017	22.632	7.122	1.00	15.96	H C
ATOM	1936	O	LEU	H	114	3.968	23.236	6.898	1.00	15.97	H O
ATOM	1937	CB	LEU	H	114	6.710	24.475	7.454	1.00	13.15	H C
ATOM	1938	CG	LEU	H	114	8.090	25.081	7.135	1.00	15.88	H C
ATOM	1939	CD1	LEU	H	114	8.406	26.194	8.129	1.00	13.86	H C
ATOM	1940	CD2	LEU	H	114	9.173	23.999	7.194	1.00	11.78	H C
ATOM	1941	N	THR	H	115	5.057	21.453	7.732	1.00	14.58	H N
ATOM	1942	CA	THR	H	115	3.846	20.791	8.197	1.00	15.14	H C
ATOM	1943	C	THR	H	115	4.087	20.219	9.591	1.00	14.81	H C
ATOM	1944	O	THR	H	115	5.158	20.404	10.168	1.00	15.34	H O
ATOM	1945	CB	THR	H	115	3.462	19.627	7.268	1.00	14.99	H C
ATOM	1946	OG1	THR	H	115	4.431	18.580	7.406	1.00	15.74	H O
ATOM	1947	CG2	THR	H	115	3.419	20.084	5.805	1.00	13.98	H C
ATOM	1948	N	ASP	H	116	3.094	19.523	10.130	1.00	15.45	H N
ATOM	1949	CA	ASP	H	116	3.244	18.904	11.437	1.00	16.55	H C
ATOM	1950	C	ASP	H	116	4.359	17.849	11.416	1.00	17.00	H C
ATOM	1951	O	ASP	H	116	4.913	17.519	12.460	1.00	16.90	H O

ATOM	1952	CB	ASP	H	116	1.934	18.244	11.883	1.00	18.41	H	C
ATOM	1953	CG	ASP	H	116	0.866	19.254	12.283	1.00	20.47	H	C
ATOM	1954	OD1	ASP	H	116	1.166	20.431	12.388	1.00	20.75	H	O
ATOM	1955	OD2	ASP	H	116	-0.270	18.844	12.496	1.00	23.70	H	O
ATOM	1956	N	HIS	H	117	4.687	17.326	10.233	1.00	15.90	H	N
ATOM	1957	CA	HIS	H	117	5.733	16.307	10.105	1.00	16.55	H	C
ATOM	1958	C	HIS	H	117	7.041	16.802	9.492	1.00	16.30	H	C
ATOM	1959	O	HIS	H	117	8.001	16.040	9.372	1.00	15.70	H	O
ATOM	1960	CB	HIS	H	117	5.217	15.115	9.297	1.00	16.16	H	C
ATOM	1961	CG	HIS	H	117	4.102	14.384	9.970	1.00	19.31	H	C
ATOM	1962	ND1	HIS	H	117	2.808	14.857	9.986	1.00	18.50	H	N
ATOM	1963	CD2	HIS	H	117	4.103	13.259	10.723	1.00	17.50	H	C
ATOM	1964	CE1	HIS	H	117	2.059	14.056	10.723	1.00	21.07	H	C
ATOM	1965	NE2	HIS	H	117	2.821	13.080	11.182	1.00	20.92	H	N
ATOM	1966	N	VAL	H	118	7.078	18.072	9.103	1.00	15.64	H	N
ATOM	1967	CA	VAL	H	118	8.276	18.655	8.511	1.00	14.14	H	C
ATOM	1968	C	VAL	H	118	8.493	20.041	9.095	1.00	14.78	H	C
ATOM	1969	O	VAL	H	118	7.784	20.984	8.762	1.00	14.27	H	O
ATOM	1970	CB	VAL	H	118	8.148	18.761	6.990	1.00	14.64	H	C
ATOM	1971	CG1	VAL	H	118	9.381	19.463	6.413	1.00	12.73	H	C
ATOM	1972	CG2	VAL	H	118	7.983	17.367	6.393	1.00	12.56	H	C
ATOM	1973	N	VAL	H	119	9.486	20.147	9.970	1.00	15.25	H	N
ATOM	1974	CA	VAL	H	119	9.808	21.394	10.653	1.00	13.86	H	C
ATOM	1975	C	VAL	H	119	11.329	21.501	10.766	1.00	14.17	H	C
ATOM	1976	O	VAL	H	119	12.017	20.499	10.956	1.00	13.56	H	O
ATOM	1977	CB	VAL	H	119	9.177	21.390	12.081	1.00	15.77	H	C
ATOM	1978	CG1	VAL	H	119	9.570	22.641	12.856	1.00	16.33	H	C
ATOM	1979	CG2	VAL	H	119	7.656	21.285	11.974	1.00	16.16	H	C
ATOM	1980	N	PRO	H	120	11.875	22.718	10.644	1.00	13.65	H	N
ATOM	1981	CA	PRO	H	120	13.325	22.881	10.746	1.00	12.56	H	C
ATOM	1982	C	PRO	H	120	13.817	22.966	12.189	1.00	13.87	H	C
ATOM	1983	O	PRO	H	120	13.085	23.398	13.086	1.00	11.70	H	O
ATOM	1984	CB	PRO	H	120	13.573	24.172	9.981	1.00	12.13	H	C
ATOM	1985	CG	PRO	H	120	12.355	24.978	10.315	1.00	15.18	H	C
ATOM	1986	CD	PRO	H	120	11.230	23.971	10.203	1.00	14.55	H	C
ATOM	1987	N	LEU	H	121	15.054	22.521	12.403	1.00	12.25	H	N
ATOM	1988	CA	LEU	H	121	15.688	22.577	13.713	1.00	11.41	H	C
ATOM	1989	C	LEU	H	121	16.359	23.944	13.719	1.00	12.91	H	C
ATOM	1990	O	LEU	H	121	16.826	24.394	12.676	1.00	12.87	H	O
ATOM	1991	CB	LEU	H	121	16.747	21.472	13.838	1.00	10.88	H	C
ATOM	1992	CG	LEU	H	121	17.592	21.380	15.124	1.00	9.26	H	C
ATOM	1993	CD1	LEU	H	121	16.692	21.104	16.320	1.00	7.01	H	C
ATOM	1994	CD2	LEU	H	121	18.640	20.259	14.978	1.00	7.10	H	C
ATOM	1995	N	CYS	H	122	16.409	24.610	14.867	1.00	13.27	H	N
ATOM	1996	CA	CYS	H	122	17.034	25.932	14.925	1.00	15.06	H	C
ATOM	1997	C	CYS	H	122	18.556	25.919	14.874	1.00	15.31	H	C
ATOM	1998	O	CYS	H	122	19.202	25.139	15.571	1.00	16.54	H	O
ATOM	1999	CB	CYS	H	122	16.657	26.684	16.205	1.00	15.03	H	C
ATOM	2000	SG	CYS	H	122	14.893	26.918	16.573	1.00	16.60	H	S
ATOM	2001	N	LEU	H	123	19.119	26.793	14.046	1.00	14.53	H	N
ATOM	2002	CA	LEU	H	123	20.560	26.955	13.970	1.00	12.48	H	C
ATOM	2003	C	LEU	H	123	20.747	28.048	15.018	1.00	12.30	H	C
ATOM	2004	O	LEU	H	123	20.207	29.149	14.876	1.00	13.28	H	O
ATOM	2005	CB	LEU	H	123	20.991	27.466	12.590	1.00	11.93	H	C
ATOM	2006	CG	LEU	H	123	22.513	27.606	12.445	1.00	12.58	H	C
ATOM	2007	CD1	LEU	H	123	23.142	26.211	12.479	1.00	9.53	H	C

ATOM	2008	CD2	LEU	H	123	22.865	28.312	11.147	1.00	10.47	H C
ATOM	2009	N	PRO	H	124	21.497	27.762	16.093	1.00	12.74	H N
ATOM	2010	CA	PRO	H	124	21.708	28.760	17.149	1.00	12.16	H C
ATOM	2011	C	PRO	H	124	22.827	29.747	16.881	1.00	13.37	H C
ATOM	2012	O	PRO	H	124	23.639	29.535	15.984	1.00	13.97	H O
ATOM	2013	CB	PRO	H	124	22.031	27.897	18.356	1.00	10.72	H C
ATOM	2014	CG	PRO	H	124	22.924	26.839	17.730	1.00	12.77	H C
ATOM	2015	CD	PRO	H	124	22.205	26.505	16.408	1.00	10.59	H C
ATOM	2016	N	GLU	H	125	22.860	30.831	17.657	1.00	13.81	H N
ATOM	2017	CA	GLU	H	125	23.947	31.800	17.533	1.00	14.83	H C
ATOM	2018	C	GLU	H	125	25.145	31.082	18.149	1.00	14.18	H C
ATOM	2019	O	GLU	H	125	24.975	30.182	18.972	1.00	13.59	H O
ATOM	2020	CB	GLU	H	125	23.656	33.085	18.319	1.00	15.94	H C
ATOM	2021	CG	GLU	H	125	22.528	33.918	17.745	1.00	20.23	H C
ATOM	2022	CD	GLU	H	125	22.427	35.292	18.380	1.00	23.56	H C
ATOM	2023	OE1	GLU	H	125	22.850	35.449	19.526	1.00	21.49	H O
ATOM	2024	OE2	GLU	H	125	21.912	36.198	17.728	1.00	25.49	H O
ATOM	2025	N	ARG	H	126	26.350	31.477	17.759	1.00	15.26	H N
ATOM	2026	CA	ARG	H	126	27.557	30.836	18.258	1.00	16.72	H C
ATOM	2027	C	ARG	H	126	27.793	30.894	19.772	1.00	16.72	H C
ATOM	2028	O	ARG	H	126	28.012	29.854	20.397	1.00	15.77	H O
ATOM	2029	CB	ARG	H	126	28.787	31.399	17.550	1.00	18.05	H C
ATOM	2030	CG	ARG	H	126	30.075	30.784	18.054	1.00	23.13	H C
ATOM	2031	CD	ARG	H	126	31.236	31.724	17.874	1.00	28.03	H C
ATOM	2032	NE	ARG	H	126	31.769	31.681	16.524	1.00	30.56	H N
ATOM	2033	CZ	ARG	H	126	32.772	30.897	16.141	1.00	33.42	H C
ATOM	2034	NH1	ARG	H	126	33.356	30.081	17.011	1.00	33.03	H N
ATOM	2035	NH2	ARG	H	126	33.199	30.945	14.886	1.00	33.65	H N
ATOM	2036	N	THR	H	127	27.764	32.086	20.365	1.00	15.89	H N
ATOM	2037	CA	THR	H	127	28.020	32.191	21.803	1.00	16.74	H C
ATOM	2038	C	THR	H	127	26.976	31.448	22.634	1.00	15.42	H C
ATOM	2039	O	THR	H	127	27.320	30.816	23.630	1.00	15.65	H O
ATOM	2040	CB	THR	H	127	28.124	33.669	22.277	1.00	19.12	H C
ATOM	2041	OG1	THR	H	127	26.860	34.323	22.127	1.00	23.54	H O
ATOM	2042	CG2	THR	H	127	29.175	34.413	21.461	1.00	18.93	H C
ATOM	2043	N	PHE	H	128	25.710	31.522	22.234	1.00	12.93	H N
ATOM	2044	CA	PHE	H	128	24.650	30.798	22.938	1.00	12.70	H C
ATOM	2045	C	PHE	H	128	25.006	29.307	22.929	1.00	11.77	H C
ATOM	2046	O	PHE	H	128	24.971	28.643	23.963	1.00	11.84	H O
ATOM	2047	CB	PHE	H	128	23.300	31.019	22.232	1.00	11.78	H C
ATOM	2048	CG	PHE	H	128	22.186	30.092	22.694	1.00	11.98	H C
ATOM	2049	CD1	PHE	H	128	21.783	30.057	24.026	1.00	13.78	H C
ATOM	2050	CD2	PHE	H	128	21.498	29.306	21.773	1.00	9.96	H C
ATOM	2051	CE1	PHE	H	128	20.704	29.256	24.437	1.00	12.05	H C
ATOM	2052	CE2	PHE	H	128	20.423	28.504	22.163	1.00	10.60	H C
ATOM	2053	CZ	PHE	H	128	20.021	28.480	23.503	1.00	12.84	H C
ATOM	2054	N	SER	H	129	25.364	28.792	21.757	1.00	11.50	H N
ATOM	2055	CA	SER	H	129	25.712	27.383	21.622	1.00	12.61	H C
ATOM	2056	C	SER	H	129	26.962	26.998	22.417	1.00	12.76	H C
ATOM	2057	O	SER	H	129	27.008	25.929	23.023	1.00	12.80	H O
ATOM	2058	CB	SER	H	129	25.908	27.029	20.145	1.00	12.21	H C
ATOM	2059	OG	SER	H	129	26.052	25.624	19.977	1.00	17.13	H O
ATOM	2060	N	GLU	H	129A	27.969	27.868	22.420	1.00	13.31	H N
ATOM	2061	CA	GLU	H	129A	29.217	27.603	23.136	1.00	14.09	H C
ATOM	2062	C	GLU	H	129A	29.128	27.730	24.657	1.00	14.85	H C
ATOM	2063	O	GLU	H	129A	29.707	26.921	25.382	1.00	14.98	H O

ATOM	2064	CB	GLU	H	129A	30.328	28.542	22.639	1.00	14.74	H	C
ATOM	2065	CG	GLU	H	129A	30.715	28.369	21.172	1.00	14.19	H	C
ATOM	2066	CD	GLU	H	129A	31.780	29.367	20.745	1.00	16.54	H	C
ATOM	2067	OE1	GLU	H	129A	31.941	30.368	21.432	1.00	16.37	H	O
ATOM	2068	OE2	GLU	H	129A	32.431	29.146	19.728	1.00	17.94	H	O
ATOM	2069	N	ARG	H	129B	28.410	28.739	25.145	1.00	15.04	H	N
ATOM	2070	CA	ARG	H	129B	28.310	28.957	26.589	1.00	16.21	H	C
ATOM	2071	C	ARG	H	129B	27.114	28.309	27.267	1.00	14.62	H	C
ATOM	2072	O	ARG	H	129B	27.124	28.110	28.479	1.00	14.82	H	O
ATOM	2073	CB	ARG	H	129B	28.296	30.460	26.904	1.00	19.47	H	C
ATOM	2074	CG	ARG	H	129B	27.031	31.161	26.451	1.00	28.02	H	C
ATOM	2075	CD	ARG	H	129B	26.919	32.605	26.946	1.00	33.00	H	C
ATOM	2076	NE	ARG	H	129B	27.978	33.478	26.447	1.00	36.47	H	N
ATOM	2077	CZ	ARG	H	129B	27.822	34.777	26.197	1.00	38.35	H	C
ATOM	2078	NH1	ARG	H	129B	26.645	35.360	26.391	1.00	38.64	H	N
ATOM	2079	NH2	ARG	H	129B	28.845	35.500	25.757	1.00	36.71	H	N
ATOM	2080	N	THR	H	129C	26.079	27.984	26.503	1.00	13.48	H	N
ATOM	2081	CA	THR	H	129C	24.897	27.378	27.094	1.00	12.08	H	C
ATOM	2082	C	THR	H	129C	24.611	25.974	26.574	1.00	12.22	H	C
ATOM	2083	O	THR	H	129C	24.631	25.021	27.344	1.00	12.56	H	O
ATOM	2084	CB	THR	H	129C	23.643	28.263	26.872	1.00	13.41	H	C
ATOM	2085	OG1	THR	H	129C	23.841	29.541	27.496	1.00	12.83	H	O
ATOM	2086	CG2	THR	H	129C	22.411	27.604	27.472	1.00	13.85	H	C
ATOM	2087	N	LEU	H	129D	24.358	25.839	25.273	1.00	9.80	H	N
ATOM	2088	CA	LEU	H	129D	24.043	24.533	24.706	1.00	9.83	H	C
ATOM	2089	C	LEU	H	129D	25.121	23.466	24.903	1.00	10.51	H	C
ATOM	2090	O	LEU	H	129D	24.802	22.292	25.092	1.00	9.04	H	O
ATOM	2091	CB	LEU	H	129D	23.717	24.661	23.215	1.00	9.11	H	C
ATOM	2092	CG	LEU	H	129D	22.473	25.482	22.856	1.00	10.83	H	C
ATOM	2093	CD1	LEU	H	129D	22.268	25.452	21.349	1.00	7.76	H	C
ATOM	2094	CD2	LEU	H	129D	21.249	24.927	23.580	1.00	8.60	H	C
ATOM	2095	N	ALA	H	129E	26.388	23.871	24.874	1.00	9.59	H	N
ATOM	2096	CA	ALA	H	129E	27.495	22.929	25.038	1.00	11.11	H	C
ATOM	2097	C	ALA	H	129E	27.527	22.284	26.417	1.00	12.05	H	C
ATOM	2098	O	ALA	H	129E	28.209	21.277	26.614	1.00	14.06	H	O
ATOM	2099	CB	ALA	H	129E	28.828	23.627	24.768	1.00	8.33	H	C
ATOM	2100	N	PHE	H	129F	26.794	22.848	27.372	1.00	11.37	H	N
ATOM	2101	CA	PHE	H	129F	26.793	22.291	28.714	1.00	11.44	H	C
ATOM	2102	C	PHE	H	129F	25.513	21.561	29.108	1.00	11.62	H	C
ATOM	2103	O	PHE	H	129F	25.328	21.163	30.260	1.00	10.42	H	O
ATOM	2104	CB	PHE	H	129F	27.180	23.386	29.714	1.00	13.71	H	C
ATOM	2105	CG	PHE	H	129F	28.562	23.937	29.469	1.00	12.82	H	C
ATOM	2106	CD1	PHE	H	129F	29.669	23.090	29.491	1.00	13.92	H	C
ATOM	2107	CD2	PHE	H	129F	28.749	25.275	29.148	1.00	13.07	H	C
ATOM	2108	CE1	PHE	H	129F	30.944	23.567	29.190	1.00	15.14	H	C
ATOM	2109	CE2	PHE	H	129F	30.017	25.765	28.844	1.00	13.32	H	C
ATOM	2110	CZ	PHE	H	129F	31.118	24.911	28.863	1.00	14.84	H	C
ATOM	2111	N	VAL	H	129G	24.633	21.380	28.132	1.00	11.71	H	N
ATOM	2112	CA	VAL	H	129G	23.418	20.617	28.339	1.00	10.87	H	C
ATOM	2113	C	VAL	H	129G	23.969	19.201	28.125	1.00	12.85	H	C
ATOM	2114	O	VAL	H	129G	24.514	18.886	27.062	1.00	12.09	H	O
ATOM	2115	CB	VAL	H	129G	22.344	20.956	27.271	1.00	10.74	H	C
ATOM	2116	CG1	VAL	H	129G	21.203	19.946	27.329	1.00	8.96	H	C
ATOM	2117	CG2	VAL	H	129G	21.806	22.372	27.510	1.00	9.81	H	C
ATOM	2118	N	ARG	H	134	23.847	18.367	29.147	1.00	12.84	H	N
ATOM	2119	CA	ARG	H	134	24.368	17.008	29.114	1.00	14.10	H	C

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ATOM   2120  C   ARG H 134      23.977  16.147  27.909  1.00 14.87      H    C
ATOM   2121  O   ARG H 134      24.831  15.767  27.104  1.00 14.59      H    O
ATOM   2122  CB  ARG H 134      23.960  16.281  30.400  1.00 14.36      H    C
ATOM   2123  CG  ARG H 134      24.450  14.840  30.485  1.00 17.60      H    C
ATOM   2124  CD  ARG H 134      25.916  14.769  30.854  1.00 20.10      H    C
ATOM   2125  NE  ARG H 134      26.154  15.328  32.182  1.00 21.14      H    N
ATOM   2126  CZ  ARG H 134      27.311  15.262  32.832  1.00 19.89      H    C
ATOM   2127  NH1 ARG H 134      28.356  14.659  32.287  1.00 20.58      H    N
ATOM   2128  NH2 ARG H 134      27.419  15.795  34.035  1.00 20.22      H    N
ATOM   2129  N   PHE H 135      22.687  15.844  27.801  1.00 12.87      H    N
ATOM   2130  CA  PHE H 135      22.164  14.986  26.745  1.00 12.91      H    C
ATOM   2131  C   PHE H 135      21.591  15.697  25.521  1.00 13.23      H    C
ATOM   2132  O   PHE H 135      21.053  16.799  25.609  1.00 15.91      H    O
ATOM   2133  CB  PHE H 135      21.089  14.054  27.340  1.00 11.61      H    C
ATOM   2134  CG  PHE H 135      21.640  12.996  28.259  1.00 11.27      H    C
ATOM   2135  CD1 PHE H 135      22.119  11.794  27.752  1.00 12.29      H    C
ATOM   2136  CD2 PHE H 135      21.694  13.205  29.631  1.00 12.45      H    C
ATOM   2137  CE1 PHE H 135      22.648  10.812  28.602  1.00 11.52      H    C
ATOM   2138  CE2 PHE H 135      22.219  12.235  30.485  1.00 13.43      H    C
ATOM   2139  CZ  PHE H 135      22.699  11.035  29.966  1.00 10.85      H    C
ATOM   2140  N   SER H 136      21.718  15.030  24.378  1.00 13.39      H    N
ATOM   2141  CA  SER H 136      21.209  15.499  23.095  1.00 13.57      H    C
ATOM   2142  C   SER H 136      20.797  14.259  22.305  1.00 13.47      H    C
ATOM   2143  O   SER H 136      21.293  13.160  22.559  1.00 11.08      H    O
ATOM   2144  CB  SER H 136      22.285  16.249  22.307  1.00 13.40      H    C
ATOM   2145  OG  SER H 136      22.576  17.513  22.881  1.00 14.55      H    O
ATOM   2146  N   LEU H 137      19.903  14.441  21.341  1.00 12.22      H    N
ATOM   2147  CA  LEU H 137      19.429  13.331  20.519  1.00 13.36      H    C
ATOM   2148  C   LEU H 137      20.157  13.217  19.187  1.00 13.34      H    C
ATOM   2149  O   LEU H 137      20.391  14.216  18.509  1.00 12.33      H    O
ATOM   2150  CB  LEU H 137      17.938  13.486  20.228  1.00 13.15      H    C
ATOM   2151  CG  LEU H 137      16.941  13.480  21.385  1.00 15.66      H    C
ATOM   2152  CD1 LEU H 137      15.532  13.692  20.815  1.00 14.08      H    C
ATOM   2153  CD2 LEU H 137      17.026  12.158  22.157  1.00 14.11      H    C
ATOM   2154  N   VAL H 138      20.524  11.991  18.827  1.00 12.73      H    N
ATOM   2155  CA  VAL H 138      21.170  11.715  17.550  1.00 12.09      H    C
ATOM   2156  C   VAL H 138      20.216  10.733  16.870  1.00 12.01      H    C
ATOM   2157  O   VAL H 138      19.675   9.836  17.513  1.00 12.12      H    O
ATOM   2158  CB  VAL H 138      22.585  11.077  17.720  1.00 13.28      H    C
ATOM   2159  CG1 VAL H 138      23.551  12.094  18.330  1.00  8.61      H    C
ATOM   2160  CG2 VAL H 138      22.506   9.842  18.600  1.00 11.66      H    C
ATOM   2161  N   SER H 139      20.002  10.897  15.573  1.00 12.22      H    N
ATOM   2162  CA  SER H 139      19.061  10.041  14.869  1.00 11.00      H    C
ATOM   2163  C   SER H 139      19.462   9.715  13.437  1.00 10.54      H    C
ATOM   2164  O   SER H 139      20.324  10.378  12.856  1.00 11.74      H    O
ATOM   2165  CB  SER H 139      17.693  10.722  14.870  1.00 11.90      H    C
ATOM   2166  OG  SER H 139      17.823  12.060  14.405  1.00  9.32      H    O
ATOM   2167  N   GLY H 140      18.818   8.690  12.881  1.00  9.70      H    N
ATOM   2168  CA  GLY H 140      19.084   8.269  11.516  1.00  9.30      H    C
ATOM   2169  C   GLY H 140      18.579   6.864  11.200  1.00  9.94      H    C
ATOM   2170  O   GLY H 140      18.082   6.147  12.076  1.00  9.85      H    O
ATOM   2171  N   TRP H 141      18.698   6.479   9.935  1.00 10.84      H    N
ATOM   2172  CA  TRP H 141      18.299   5.149   9.471  1.00 13.57      H    C
ATOM   2173  C   TRP H 141      19.547   4.284   9.307  1.00 14.42      H    C
ATOM   2174  O   TRP H 141      19.559   3.338   8.518  1.00 14.11      H    O
ATOM   2175  CB  TRP H 141      17.585   5.251   8.119  1.00 11.62      H    C
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ATOM	2176	CG	TRP	H	141	16.213	5.852	8.198	1.00	9.53	H C
ATOM	2177	CD1	TRP	H	141	15.042	5.194	8.451	1.00	7.95	H C
ATOM	2178	CD2	TRP	H	141	15.868	7.227	7.992	1.00	9.12	H C
ATOM	2179	NE1	TRP	H	141	13.987	6.076	8.407	1.00	10.35	H N
ATOM	2180	CE2	TRP	H	141	14.465	7.330	8.131	1.00	9.30	H C
ATOM	2181	CE3	TRP	H	141	16.609	8.381	7.700	1.00	6.96	H C
ATOM	2182	CZ2	TRP	H	141	13.784	8.547	7.992	1.00	9.43	H C
ATOM	2183	CZ3	TRP	H	141	15.934	9.590	7.559	1.00	8.75	H C
ATOM	2184	CH2	TRP	H	141	14.531	9.662	7.707	1.00	9.90	H C
ATOM	2185	N	GLY	H	142	20.591	4.623	10.059	1.00	16.02	H N
ATOM	2186	CA	GLY	H	142	21.848	3.898	9.988	1.00	15.99	H C
ATOM	2187	C	GLY	H	142	21.825	2.514	10.589	1.00	15.07	H C
ATOM	2188	O	GLY	H	142	20.767	2.010	10.972	1.00	15.13	H O
ATOM	2189	N	GLN	H	143	23.006	1.904	10.672	1.00	16.63	H N
ATOM	2190	CA	GLN	H	143	23.162	0.556	11.212	1.00	17.93	H C
ATOM	2191	C	GLN	H	143	22.665	0.409	12.640	1.00	20.58	H C
ATOM	2192	O	GLN	H	143	22.882	1.278	13.489	1.00	18.31	H O
ATOM	2193	CB	GLN	H	143	24.628	0.110	11.167	1.00	18.10	H C
ATOM	2194	CG	GLN	H	143	25.228	-0.100	9.770	1.00	19.46	H C
ATOM	2195	CD	GLN	H	143	25.525	1.199	9.043	1.00	21.99	H C
ATOM	2196	OE1	GLN	H	143	25.714	2.242	9.669	1.00	20.13	H O
ATOM	2197	NE2	GLN	H	143	25.588	1.137	7.712	1.00	20.26	H N
ATOM	2198	N	LEU	H	144	22.003	-0.714	12.898	1.00	21.01	H N
ATOM	2199	CA	LEU	H	144	21.481	-1.012	14.221	1.00	23.46	H C
ATOM	2200	C	LEU	H	144	22.573	-1.658	15.069	1.00	25.89	H C
ATOM	2201	O	LEU	H	144	22.507	-1.642	16.298	1.00	25.66	H O
ATOM	2202	CB	LEU	H	144	20.269	-1.944	14.101	1.00	21.41	H C
ATOM	2203	CG	LEU	H	144	19.080	-1.313	13.367	1.00	19.40	H C
ATOM	2204	CD1	LEU	H	144	17.980	-2.352	13.121	1.00	21.44	H C
ATOM	2205	CD2	LEU	H	144	18.551	-0.157	14.199	1.00	14.43	H C
ATOM	2206	N	LEU	H	145	23.574	-2.226	14.400	1.00	27.35	H N
ATOM	2207	CA	LEU	H	145	24.700	-2.875	15.067	1.00	32.19	H C
ATOM	2208	C	LEU	H	145	25.976	-2.620	14.267	1.00	32.79	H C
ATOM	2209	O	LEU	H	145	25.916	-2.351	13.067	1.00	33.17	H O
ATOM	2210	CB	LEU	H	145	24.470	-4.391	15.186	1.00	33.26	H C
ATOM	2211	CG	LEU	H	145	23.588	-4.949	16.311	1.00	35.26	H C
ATOM	2212	CD1	LEU	H	145	22.133	-4.554	16.123	1.00	37.31	H C
ATOM	2213	CD2	LEU	H	145	23.704	-6.456	16.313	1.00	36.17	H C
ATOM	2214	N	ASP	H	146	27.124	-2.694	14.934	1.00	33.83	H N
ATOM	2215	CA	ASP	H	146	28.404	-2.483	14.266	1.00	35.01	H C
ATOM	2216	C	ASP	H	146	28.493	-3.449	13.091	1.00	36.95	H C
ATOM	2217	O	ASP	H	146	28.380	-4.661	13.268	1.00	36.80	H O
ATOM	2218	CB	ASP	H	146	29.562	-2.750	15.232	1.00	35.30	H C
ATOM	2219	CG	ASP	H	146	30.922	-2.459	14.612	1.00	35.18	H C
ATOM	2220	OD1	ASP	H	146	31.245	-1.297	14.431	1.00	33.00	H O
ATOM	2221	OD2	ASP	H	146	31.652	-3.406	14.310	1.00	36.91	H O
ATOM	2222	N	ARG	H	147	28.679	-2.906	11.893	1.00	38.24	H N
ATOM	2223	CA	ARG	H	147	28.782	-3.719	10.686	1.00	40.29	H C
ATOM	2224	C	ARG	H	147	27.507	-4.535	10.434	1.00	39.24	H C
ATOM	2225	O	ARG	H	147	27.550	-5.613	9.842	1.00	40.33	H O
ATOM	2226	CB	ARG	H	147	29.995	-4.651	10.797	1.00	43.36	H C
ATOM	2227	CG	ARG	H	147	30.348	-5.385	9.516	1.00	48.53	H C
ATOM	2228	CD	ARG	H	147	31.593	-6.237	9.598	1.00	54.02	H C
ATOM	2229	NE	ARG	H	147	31.930	-6.977	8.484	1.00	56.36	H N
ATOM	2230	CZ	ARG	H	147	32.980	-7.784	8.361	1.00	58.31	H C
ATOM	2231	NH1	ARG	H	147	33.811	-7.965	9.381	1.00	58.01	H N

ATOM	2232	NH2	ARG	H	147	33.199	-8.414	7.215	1.00	58.04	H	N
ATOM	2233	N	GLY	H	149	26.372	-4.009	10.883	1.00	36.85	H	N
ATOM	2234	CA	GLY	H	149	25.109	-4.696	10.697	1.00	33.07	H	C
ATOM	2235	C	GLY	H	149	24.277	-4.049	9.610	1.00	30.38	H	C
ATOM	2236	O	GLY	H	149	24.782	-3.246	8.826	1.00	29.52	H	O
ATOM	2237	N	ALA	H	150	22.997	-4.398	9.562	1.00	28.41	H	N
ATOM	2238	CA	ALA	H	150	22.091	-3.846	8.561	1.00	26.03	H	C
ATOM	2239	C	ALA	H	150	21.468	-2.542	9.048	1.00	23.50	H	C
ATOM	2240	O	ALA	H	150	21.415	-2.283	10.249	1.00	21.67	H	O
ATOM	2241	CB	ALA	H	150	21.005	-4.850	8.248	1.00	27.18	H	C
ATOM	2242	N	THR	H	151	20.986	-1.732	8.112	1.00	22.99	H	N
ATOM	2243	CA	THR	H	151	20.374	-0.455	8.458	1.00	22.82	H	C
ATOM	2244	C	THR	H	151	18.923	-0.593	8.925	1.00	22.79	H	C
ATOM	2245	O	THR	H	151	18.302	-1.651	8.783	1.00	21.21	H	O
ATOM	2246	CB	THR	H	151	20.450	0.538	7.278	1.00	23.93	H	C
ATOM	2247	OG1	THR	H	151	19.822	-0.027	6.122	1.00	22.56	H	O
ATOM	2248	CG2	THR	H	151	21.903	0.865	6.956	1.00	22.44	H	C
ATOM	2249	N	ALA	H	152	18.389	0.484	9.493	1.00	20.52	H	N
ATOM	2250	CA	ALA	H	152	17.025	0.474	10.005	1.00	18.60	H	C
ATOM	2251	C	ALA	H	152	15.979	0.962	9.011	1.00	16.25	H	C
ATOM	2252	O	ALA	H	152	16.218	1.883	8.237	1.00	16.12	H	O
ATOM	2253	CB	ALA	H	152	16.951	1.303	11.280	1.00	18.25	H	C
ATOM	2254	N	LEU	H	153	14.811	0.332	9.045	1.00	15.23	H	N
ATOM	2255	CA	LEU	H	153	13.713	0.707	8.169	1.00	15.57	H	C
ATOM	2256	C	LEU	H	153	12.954	1.881	8.754	1.00	14.76	H	C
ATOM	2257	O	LEU	H	153	12.443	2.720	8.021	1.00	17.16	H	O
ATOM	2258	CB	LEU	H	153	12.770	-0.479	7.962	1.00	15.57	H	C
ATOM	2259	CG	LEU	H	153	13.349	-1.531	7.015	1.00	16.60	H	C
ATOM	2260	CD1	LEU	H	153	12.575	-2.847	7.125	1.00	16.63	H	C
ATOM	2261	CD2	LEU	H	153	13.302	-0.978	5.602	1.00	15.24	H	C
ATOM	2262	N	GLU	H	154	12.871	1.933	10.079	1.00	15.00	H	N
ATOM	2263	CA	GLU	H	154	12.182	3.025	10.755	1.00	15.61	H	C
ATOM	2264	C	GLU	H	154	13.198	3.936	11.431	1.00	14.97	H	C
ATOM	2265	O	GLU	H	154	14.143	3.465	12.070	1.00	15.21	H	O
ATOM	2266	CB	GLU	H	154	11.201	2.482	11.789	1.00	14.17	H	C
ATOM	2267	CG	GLU	H	154	9.877	2.027	11.206	1.00	20.51	H	C
ATOM	2268	CD	GLU	H	154	8.914	1.551	12.274	1.00	23.96	H	C
ATOM	2269	OE1	GLU	H	154	9.164	0.504	12.851	1.00	23.53	H	O
ATOM	2270	OE2	GLU	H	154	7.919	2.249	12.535	1.00	27.22	H	O
ATOM	2271	N	LEU	H	155	13.000	5.241	11.279	1.00	14.72	H	N
ATOM	2272	CA	LEU	H	155	13.900	6.234	11.864	1.00	13.82	H	C
ATOM	2273	C	LEU	H	155	14.157	5.954	13.336	1.00	12.35	H	C
ATOM	2274	O	LEU	H	155	13.223	5.883	14.127	1.00	13.95	H	O
ATOM	2275	CB	LEU	H	155	13.304	7.635	11.725	1.00	14.43	H	C
ATOM	2276	CG	LEU	H	155	14.144	8.775	12.315	1.00	13.63	H	C
ATOM	2277	CD1	LEU	H	155	15.464	8.868	11.565	1.00	13.84	H	C
ATOM	2278	CD2	LEU	H	155	13.380	10.088	12.210	1.00	13.06	H	C
ATOM	2279	N	MET	H	156	15.424	5.805	13.701	1.00	12.83	H	N
ATOM	2280	CA	MET	H	156	15.798	5.542	15.087	1.00	12.93	H	C
ATOM	2281	C	MET	H	156	16.366	6.812	15.739	1.00	12.73	H	C
ATOM	2282	O	MET	H	156	16.871	7.700	15.054	1.00	13.04	H	O
ATOM	2283	CB	MET	H	156	16.841	4.421	15.150	1.00	12.00	H	C
ATOM	2284	CG	MET	H	156	16.461	3.125	14.429	1.00	12.49	H	C
ATOM	2285	SD	MET	H	156	15.054	2.200	15.133	1.00	13.73	H	S
ATOM	2286	CE	MET	H	156	15.766	1.648	16.690	1.00	12.82	H	C
ATOM	2287	N	VAL	H	157	16.292	6.883	17.066	1.00	12.85	H	N

ATOM	2288	CA	VAL	H	157	16.779	8.037	17.813	1.00	11.88	H C
ATOM	2289	C	VAL	H	157	17.463	7.558	19.098	1.00	13.44	H C
ATOM	2290	O	VAL	H	157	17.127	6.499	19.642	1.00	12.26	H O
ATOM	2291	CB	VAL	H	157	15.606	9.020	18.126	1.00	9.61	H C
ATOM	2292	CG1	VAL	H	157	14.621	8.382	19.074	1.00	9.52	H C
ATOM	2293	CG2	VAL	H	157	16.142	10.337	18.685	1.00	11.73	H C
ATOM	2294	N	LEU	H	158	18.425	8.343	19.574	1.00	12.79	H N
ATOM	2295	CA	LEU	H	158	19.202	7.999	20.758	1.00	11.41	H C
ATOM	2296	C	LEU	H	158	19.660	9.223	21.545	1.00	13.56	H C
ATOM	2297	O	LEU	H	158	20.119	10.215	20.963	1.00	10.13	H O
ATOM	2298	CB	LEU	H	158	20.444	7.215	20.331	1.00	12.58	H C
ATOM	2299	CG	LEU	H	158	21.465	6.879	21.414	1.00	11.97	H C
ATOM	2300	CD1	LEU	H	158	20.871	5.843	22.360	1.00	11.50	H C
ATOM	2301	CD2	LEU	H	158	22.740	6.350	20.770	1.00	11.54	H C
ATOM	2302	N	ASN	H	159	19.547	9.138	22.869	1.00	11.48	H N
ATOM	2303	CA	ASN	H	159	19.973	10.216	23.749	1.00	13.66	H C
ATOM	2304	C	ASN	H	159	21.419	9.908	24.142	1.00	12.37	H C
ATOM	2305	O	ASN	H	159	21.701	8.835	24.673	1.00	13.12	H O
ATOM	2306	CB	ASN	H	159	19.092	10.254	25.004	1.00	15.32	H C
ATOM	2307	CG	ASN	H	159	19.000	11.643	25.621	1.00	18.58	H C
ATOM	2308	OD1	ASN	H	159	18.609	11.791	26.783	1.00	19.52	H O
ATOM	2309	ND2	ASN	H	159	19.341	12.668	24.843	1.00	17.35	H N
ATOM	2310	N	VAL	H	160	22.331	10.835	23.867	1.00	11.23	H N
ATOM	2311	CA	VAL	H	160	23.741	10.644	24.196	1.00	10.26	H C
ATOM	2312	C	VAL	H	160	24.309	11.844	24.952	1.00	11.62	H C
ATOM	2313	O	VAL	H	160	23.965	12.989	24.658	1.00	11.36	H O
ATOM	2314	CB	VAL	H	160	24.608	10.425	22.926	1.00	11.37	H C
ATOM	2315	CG1	VAL	H	160	24.175	9.147	22.200	1.00	9.21	H C
ATOM	2316	CG2	VAL	H	160	24.506	11.650	21.989	1.00	7.47	H C
ATOM	2317	N	PRO	H	161	25.183	11.590	25.947	1.00	10.82	H N
ATOM	2318	CA	PRO	H	161	25.804	12.652	26.746	1.00	11.11	H C
ATOM	2319	C	PRO	H	161	27.055	13.199	26.058	1.00	10.16	H C
ATOM	2320	O	PRO	H	161	27.822	12.458	25.445	1.00	9.67	H O
ATOM	2321	CB	PRO	H	161	26.129	11.944	28.058	1.00	10.26	H C
ATOM	2322	CG	PRO	H	161	26.562	10.594	27.575	1.00	10.20	H C
ATOM	2323	CD	PRO	H	161	25.505	10.264	26.511	1.00	11.31	H C
ATOM	2324	N	ARG	H	162	27.268	14.499	26.185	1.00	10.55	H N
ATOM	2325	CA	ARG	H	162	28.411	15.145	25.560	1.00	10.54	H C
ATOM	2326	C	ARG	H	162	29.639	15.171	26.474	1.00	11.25	H C
ATOM	2327	O	ARG	H	162	29.515	15.158	27.701	1.00	13.29	H O
ATOM	2328	CB	ARG	H	162	28.004	16.564	25.152	1.00	11.25	H C
ATOM	2329	CG	ARG	H	162	29.082	17.391	24.464	1.00	12.83	H C
ATOM	2330	CD	ARG	H	162	28.483	18.669	23.889	1.00	9.42	H C
ATOM	2331	NE	ARG	H	162	29.498	19.534	23.303	1.00	9.59	H N
ATOM	2332	CZ	ARG	H	162	29.236	20.576	22.520	1.00	11.68	H C
ATOM	2333	NH1	ARG	H	162	27.979	20.886	22.217	1.00	11.81	H N
ATOM	2334	NH2	ARG	H	162	30.232	21.318	22.047	1.00	12.43	H N
ATOM	2335	N	LEU	H	163	30.825	15.178	25.872	1.00	9.08	H N
ATOM	2336	CA	LEU	H	163	32.062	15.230	26.636	1.00	10.57	H C
ATOM	2337	C	LEU	H	163	32.991	16.323	26.127	1.00	11.95	H C
ATOM	2338	O	LEU	H	163	33.074	16.570	24.923	1.00	10.27	H O
ATOM	2339	CB	LEU	H	163	32.835	13.907	26.548	1.00	12.13	H C
ATOM	2340	CG	LEU	H	163	32.369	12.650	27.278	1.00	12.88	H C
ATOM	2341	CD1	LEU	H	163	31.177	12.034	26.547	1.00	12.78	H C
ATOM	2342	CD2	LEU	H	163	33.540	11.658	27.336	1.00	14.29	H C
ATOM	2343	N	MET	H	164	33.677	16.990	27.047	1.00	11.82	H N

ATOM	2344	CA	MET	H	164	34.654	17.980	26.633	1.00	12.80	H C
ATOM	2345	C	MET	H	164	35.782	17.109	26.081	1.00	12.63	H C
ATOM	2346	O	MET	H	164	35.980	15.977	26.532	1.00	10.67	H O
ATOM	2347	CB	MET	H	164	35.107	18.825	27.822	1.00	14.08	H C
ATOM	2348	CG	MET	H	164	34.020	19.805	28.259	1.00	18.16	H C
ATOM	2349	SD	MET	H	164	34.564	21.069	29.400	1.00	22.97	H S
ATOM	2350	CE	MET	H	164	35.402	22.150	28.252	1.00	19.99	H C
ATOM	2351	N	THR	H	165	36.504	17.621	25.095	1.00	12.59	H N
ATOM	2352	CA	THR	H	165	37.554	16.849	24.451	1.00	15.62	H C
ATOM	2353	C	THR	H	165	38.629	16.275	25.375	1.00	16.25	H C
ATOM	2354	O	THR	H	165	39.064	15.143	25.186	1.00	15.20	H O
ATOM	2355	CB	THR	H	165	38.172	17.679	23.320	1.00	17.38	H C
ATOM	2356	OG1	THR	H	165	37.112	18.103	22.452	1.00	17.32	H O
ATOM	2357	CG2	THR	H	165	39.175	16.855	22.510	1.00	14.61	H C
ATOM	2358	N	GLN	H	166	39.048	17.036	26.378	1.00	16.53	H N
ATOM	2359	CA	GLN	H	166	40.055	16.541	27.310	1.00	17.06	H C
ATOM	2360	C	GLN	H	166	39.549	15.231	27.923	1.00	17.05	H C
ATOM	2361	O	GLN	H	166	40.284	14.250	28.008	1.00	16.97	H O
ATOM	2362	CB	GLN	H	166	40.316	17.585	28.400	1.00	16.34	H C
ATOM	2363	CG	GLN	H	166	41.362	17.196	29.432	1.00	18.36	H C
ATOM	2364	CD	GLN	H	166	41.681	18.350	30.373	1.00	18.67	H C
ATOM	2365	OE1	GLN	H	166	42.310	19.329	29.973	1.00	22.60	H O
ATOM	2366	NE2	GLN	H	166	41.228	18.249	31.618	1.00	14.45	H N
ATOM	2367	N	ASP	H	167	38.290	15.217	28.347	1.00	17.30	H N
ATOM	2368	CA	ASP	H	167	37.707	14.010	28.916	1.00	17.76	H C
ATOM	2369	C	ASP	H	167	37.628	12.893	27.876	1.00	17.98	H C
ATOM	2370	O	ASP	H	167	37.922	11.739	28.182	1.00	18.09	H O
ATOM	2371	CB	ASP	H	167	36.302	14.282	29.456	1.00	18.74	H C
ATOM	2372	CG	ASP	H	167	36.313	15.086	30.729	1.00	18.60	H C
ATOM	2373	OD1	ASP	H	167	37.056	14.726	31.625	1.00	19.37	H O
ATOM	2374	OD2	ASP	H	167	35.569	16.071	30.818	1.00	20.49	H O
ATOM	2375	N	CYS	H	168	37.226	13.227	26.651	1.00	17.56	H N
ATOM	2376	CA	CYS	H	168	37.114	12.210	25.608	1.00	18.06	H C
ATOM	2377	C	CYS	H	168	38.449	11.496	25.398	1.00	18.33	H C
ATOM	2378	O	CYS	H	168	38.508	10.270	25.404	1.00	17.46	H O
ATOM	2379	CB	CYS	H	168	36.658	12.829	24.281	1.00	17.54	H C
ATOM	2380	SG	CYS	H	168	36.253	11.592	23.003	1.00	18.27	H S
ATOM	2381	N	LEU	H	169	39.511	12.271	25.202	1.00	18.38	H N
ATOM	2382	CA	LEU	H	169	40.843	11.711	24.990	1.00	22.32	H C
ATOM	2383	C	LEU	H	169	41.294	10.864	26.175	1.00	23.09	H C
ATOM	2384	O	LEU	H	169	41.797	9.757	25.995	1.00	23.96	H O
ATOM	2385	CB	LEU	H	169	41.861	12.830	24.748	1.00	22.08	H C
ATOM	2386	CG	LEU	H	169	41.665	13.649	23.471	1.00	24.49	H C
ATOM	2387	CD1	LEU	H	169	42.705	14.766	23.403	1.00	24.94	H C
ATOM	2388	CD2	LEU	H	169	41.779	12.733	22.260	1.00	23.41	H C
ATOM	2389	N	GLN	H	170	41.103	11.377	27.386	1.00	22.94	H N
ATOM	2390	CA	GLN	H	170	41.508	10.651	28.584	1.00	24.75	H C
ATOM	2391	C	GLN	H	170	40.732	9.350	28.756	1.00	26.16	H C
ATOM	2392	O	GLN	H	170	41.298	8.337	29.161	1.00	26.39	H O
ATOM	2393	CB	GLN	H	170	41.333	11.532	29.837	1.00	21.09	H C
ATOM	2394	CG	GLN	H	170	42.137	12.840	29.793	1.00	20.61	H C
ATOM	2395	CD	GLN	H	170	42.114	13.623	31.103	1.00	19.91	H C
ATOM	2396	OE1	GLN	H	170	41.153	13.560	31.874	1.00	19.12	H O
ATOM	2397	NE2	GLN	H	170	43.174	14.382	31.348	1.00	16.44	H N
ATOM	2398	N	GLN	H	170A	39.442	9.379	28.432	1.00	26.53	H N
ATOM	2399	CA	GLN	H	170A	38.576	8.210	28.572	1.00	26.34	H C

ATOM	2400	C	GLN	H	170A	38.536	7.266	27.371	1.00	26.09	H C
ATOM	2401	O	GLN	H	170A	37.795	6.288	27.386	1.00	26.50	H O
ATOM	2402	CB	GLN	H	170A	37.146	8.655	28.884	1.00	28.29	H C
ATOM	2403	CG	GLN	H	170A	36.957	9.298	30.236	1.00	30.52	H C
ATOM	2404	CD	GLN	H	170A	35.513	9.682	30.478	1.00	34.79	H C
ATOM	2405	OE1	GLN	H	170A	34.602	8.867	30.290	1.00	37.17	H O
ATOM	2406	NE2	GLN	H	170A	35.290	10.921	30.904	1.00	34.78	H N
ATOM	2407	N	SER	H	170B	39.317	7.549	26.336	1.00	26.18	H N
ATOM	2408	CA	SER	H	170B	39.317	6.696	25.159	1.00	28.66	H C
ATOM	2409	C	SER	H	170B	40.585	5.848	25.055	1.00	31.18	H C
ATOM	2410	O	SER	H	170B	41.643	6.231	25.552	1.00	29.81	H O
ATOM	2411	CB	SER	H	170B	39.153	7.544	23.890	1.00	27.91	H C
ATOM	2412	OG	SER	H	170B	37.912	8.239	23.886	1.00	24.13	H O
ATOM	2413	N	ARG	H	170C	40.459	4.688	24.417	1.00	33.34	H N
ATOM	2414	CA	ARG	H	170C	41.579	3.777	24.211	1.00	36.91	H C
ATOM	2415	C	ARG	H	170C	42.471	4.323	23.102	1.00	38.48	H C
ATOM	2416	O	ARG	H	170C	42.078	4.341	21.939	1.00	39.23	H O
ATOM	2417	CB	ARG	H	170C	41.059	2.395	23.805	1.00	37.94	H C
ATOM	2418	CG	ARG	H	170C	40.558	1.530	24.947	1.00	38.36	H C
ATOM	2419	CD	ARG	H	170C	41.710	0.756	25.572	1.00	39.49	H C
ATOM	2420	NE	ARG	H	170C	42.369	-0.108	24.592	1.00	39.64	H N
ATOM	2421	CZ	ARG	H	170C	41.864	-1.246	24.122	1.00	40.03	H C
ATOM	2422	NH1	ARG	H	170C	40.684	-1.686	24.540	1.00	41.69	H N
ATOM	2423	NH2	ARG	H	170C	42.540	-1.941	23.217	1.00	41.52	H N
ATOM	2424	N	LYS	H	170D	43.670	4.765	23.459	1.00	41.25	H N
ATOM	2425	CA	LYS	H	170D	44.605	5.306	22.472	1.00	43.27	H C
ATOM	2426	C	LYS	H	170D	44.971	4.266	21.415	1.00	44.63	H C
ATOM	2427	O	LYS	H	170D	45.314	3.137	21.752	1.00	45.60	H O
ATOM	2428	CB	LYS	H	170D	45.876	5.790	23.170	1.00	44.06	H C
ATOM	2429	CG	LYS	H	170D	45.660	6.974	24.098	1.00	43.63	H C
ATOM	2430	CD	LYS	H	170D	45.336	8.243	23.320	1.00	43.73	H C
ATOM	2431	CE	LYS	H	170D	44.179	8.998	23.957	1.00	42.88	H C
ATOM	2432	NZ	LYS	H	170D	42.919	8.196	23.891	1.00	44.55	H N
ATOM	2433	N	VAL	H	170E	44.897	4.647	20.141	1.00	45.92	H N
ATOM	2434	CA	VAL	H	170E	45.229	3.737	19.050	1.00	47.38	H C
ATOM	2435	C	VAL	H	170E	46.174	4.403	18.038	1.00	48.37	H C
ATOM	2436	O	VAL	H	170E	46.307	5.628	18.008	1.00	48.59	H O
ATOM	2437	CB	VAL	H	170E	43.955	3.237	18.317	1.00	48.27	H C
ATOM	2438	CG1	VAL	H	170E	43.053	2.478	19.283	1.00	48.47	H C
ATOM	2439	CG2	VAL	H	170E	43.195	4.398	17.721	1.00	50.40	H C
ATOM	2440	N	GLY	H	170F	46.828	3.580	17.220	1.00	49.26	H N
ATOM	2441	CA	GLY	H	170F	47.778	4.055	16.227	1.00	49.68	H C
ATOM	2442	C	GLY	H	170F	47.456	5.293	15.409	1.00	49.19	H C
ATOM	2443	O	GLY	H	170F	47.643	6.420	15.869	1.00	49.83	H O
ATOM	2444	N	ASP	H	170G	46.988	5.081	14.181	1.00	49.28	H N
ATOM	2445	CA	ASP	H	170G	46.666	6.176	13.262	1.00	48.00	H C
ATOM	2446	C	ASP	H	170G	45.293	6.803	13.484	1.00	44.35	H C
ATOM	2447	O	ASP	H	170G	44.613	7.177	12.527	1.00	44.23	H O
ATOM	2448	CB	ASP	H	170G	46.771	5.684	11.815	1.00	52.87	H C
ATOM	2449	CG	ASP	H	170G	48.206	5.571	11.341	1.00	56.13	H C
ATOM	2450	OD1	ASP	H	170G	48.987	4.862	11.981	1.00	59.14	H O
ATOM	2451	OD2	ASP	H	170G	48.545	6.193	10.325	1.00	58.70	H O
ATOM	2452	N	SER	H	170H	44.899	6.933	14.745	1.00	39.99	H N
ATOM	2453	CA	SER	H	170H	43.613	7.524	15.084	1.00	36.53	H C
ATOM	2454	C	SER	H	170H	43.583	9.003	14.727	1.00	32.15	H C
ATOM	2455	O	SER	H	170H	44.501	9.747	15.056	1.00	31.87	H O

ATOM	2456	CB	SER H 170H	43.337	7.364	16.579	1.00	37.95	H	C
ATOM	2457	OG	SER H 170H	42.120	7.987	16.949	1.00	42.60	H	O
ATOM	2458	N	PRO H 170I	42.529	9.442	14.026	1.00	28.54	H	N
ATOM	2459	CA	PRO H 170I	42.433	10.856	13.660	1.00	26.44	H	C
ATOM	2460	C	PRO H 170I	42.405	11.701	14.931	1.00	25.04	H	C
ATOM	2461	O	PRO H 170I	41.964	11.239	15.981	1.00	24.79	H	O
ATOM	2462	CB	PRO H 170I	41.112	10.921	12.900	1.00	24.88	H	C
ATOM	2463	CG	PRO H 170I	41.032	9.575	12.255	1.00	26.28	H	C
ATOM	2464	CD	PRO H 170I	41.466	8.658	13.376	1.00	26.49	H	C
ATOM	2465	N	ASN H 175	42.890	12.930	14.842	1.00	24.55	H	N
ATOM	2466	CA	ASN H 175	42.884	13.820	15.994	1.00	24.55	H	C
ATOM	2467	C	ASN H 175	41.484	14.376	16.174	1.00	21.18	H	C
ATOM	2468	O	ASN H 175	40.733	14.509	15.211	1.00	19.35	H	O
ATOM	2469	CB	ASN H 175	43.839	15.004	15.788	1.00	26.79	H	C
ATOM	2470	CG	ASN H 175	45.269	14.576	15.576	1.00	30.83	H	C
ATOM	2471	OD1	ASN H 175	45.829	13.823	16.370	1.00	32.43	H	O
ATOM	2472	ND2	ASN H 175	45.876	15.064	14.499	1.00	33.68	H	N
ATOM	2473	N	ILE H 176	41.140	14.695	17.414	1.00	18.30	H	N
ATOM	2474	CA	ILE H 176	39.852	15.290	17.716	1.00	17.01	H	C
ATOM	2475	C	ILE H 176	40.181	16.773	17.786	1.00	17.25	H	C
ATOM	2476	O	ILE H 176	40.800	17.232	18.740	1.00	18.43	H	O
ATOM	2477	CB	ILE H 176	39.306	14.807	19.077	1.00	16.65	H	C
ATOM	2478	CG1	ILE H 176	39.186	13.277	19.073	1.00	15.60	H	C
ATOM	2479	CG2	ILE H 176	37.935	15.437	19.343	1.00	13.67	H	C
ATOM	2480	CD1	ILE H 176	38.827	12.685	20.411	1.00	17.27	H	C
ATOM	2481	N	THR H 177	39.784	17.521	16.764	1.00	16.30	H	N
ATOM	2482	CA	THR H 177	40.094	18.945	16.712	1.00	15.04	H	C
ATOM	2483	C	THR H 177	39.060	19.829	17.400	1.00	14.07	H	C
ATOM	2484	O	THR H 177	38.107	19.344	18.006	1.00	13.41	H	O
ATOM	2485	CB	THR H 177	40.227	19.419	15.258	1.00	16.10	H	C
ATOM	2486	OG1	THR H 177	38.926	19.445	14.655	1.00	16.94	H	O
ATOM	2487	CG2	THR H 177	41.149	18.479	14.460	1.00	12.71	H	C
ATOM	2488	N	GLU H 178	39.266	21.138	17.305	1.00	13.19	H	N
ATOM	2489	CA	GLU H 178	38.351	22.106	17.893	1.00	14.78	H	C
ATOM	2490	C	GLU H 178	37.062	22.188	17.074	1.00	13.86	H	C
ATOM	2491	O	GLU H 178	36.104	22.847	17.478	1.00	12.84	H	O
ATOM	2492	CB	GLU H 178	39.009	23.490	17.955	1.00	18.37	H	C
ATOM	2493	CG	GLU H 178	39.254	24.129	16.596	1.00	20.75	H	C
ATOM	2494	CD	GLU H 178	40.674	23.943	16.096	1.00	27.62	H	C
ATOM	2495	OE1	GLU H 178	41.148	22.778	16.008	1.00	27.54	H	O
ATOM	2496	OE2	GLU H 178	41.317	24.969	15.785	1.00	30.43	H	O
ATOM	2497	N	TYR H 179	37.044	21.524	15.921	1.00	12.57	H	N
ATOM	2498	CA	TYR H 179	35.868	21.517	15.056	1.00	11.69	H	C
ATOM	2499	C	TYR H 179	35.042	20.248	15.265	1.00	11.04	H	C
ATOM	2500	O	TYR H 179	34.189	19.910	14.444	1.00	11.12	H	O
ATOM	2501	CB	TYR H 179	36.317	21.637	13.594	1.00	12.21	H	C
ATOM	2502	CG	TYR H 179	37.076	22.924	13.342	1.00	15.01	H	C
ATOM	2503	CD1	TYR H 179	36.406	24.148	13.311	1.00	13.28	H	C
ATOM	2504	CD2	TYR H 179	38.466	22.927	13.211	1.00	13.16	H	C
ATOM	2505	CE1	TYR H 179	37.090	25.344	13.163	1.00	15.33	H	C
ATOM	2506	CE2	TYR H 179	39.169	24.124	13.062	1.00	16.25	H	C
ATOM	2507	CZ	TYR H 179	38.468	25.329	13.043	1.00	17.14	H	C
ATOM	2508	OH	TYR H 179	39.134	26.519	12.935	1.00	17.38	H	O
ATOM	2509	N	MET H 180	35.289	19.567	16.383	1.00	11.28	H	N
ATOM	2510	CA	MET H 180	34.607	18.319	16.711	1.00	10.08	H	C
ATOM	2511	C	MET H 180	34.345	18.230	18.210	1.00	10.42	H	C

ATOM	2512	O	MET	H	180	34.873	19.014	18.992	1.00	11.63	H	O
ATOM	2513	CB	MET	H	180	35.498	17.122	16.359	1.00	10.13	H	C
ATOM	2514	CG	MET	H	180	36.249	17.191	15.046	1.00	11.90	H	C
ATOM	2515	SD	MET	H	180	37.417	15.806	14.948	1.00	13.02	H	S
ATOM	2516	CE	MET	H	180	38.056	16.055	13.327	1.00	10.31	H	C
ATOM	2517	N	PHE	H	181	33.544	17.246	18.603	1.00	10.40	H	N
ATOM	2518	CA	PHE	H	181	33.276	16.987	20.012	1.00	10.41	H	C
ATOM	2519	C	PHE	H	181	32.745	15.564	20.107	1.00	11.92	H	C
ATOM	2520	O	PHE	H	181	32.119	15.070	19.167	1.00	11.21	H	O
ATOM	2521	CB	PHE	H	181	32.293	18.010	20.600	1.00	10.04	H	C
ATOM	2522	CG	PHE	H	181	30.857	17.822	20.179	1.00	11.23	H	C
ATOM	2523	CD1	PHE	H	181	30.057	16.852	20.784	1.00	9.00	H	C
ATOM	2524	CD2	PHE	H	181	30.292	18.650	19.210	1.00	10.30	H	C
ATOM	2525	CE1	PHE	H	181	28.712	16.711	20.434	1.00	10.61	H	C
ATOM	2526	CE2	PHE	H	181	28.941	18.518	18.848	1.00	9.40	H	C
ATOM	2527	CZ	PHE	H	181	28.152	17.548	19.464	1.00	9.56	H	C
ATOM	2528	N	CYS	H	182	33.030	14.892	21.217	1.00	11.17	H	N
ATOM	2529	CA	CYS	H	182	32.576	13.525	21.408	1.00	13.43	H	C
ATOM	2530	C	CYS	H	182	31.306	13.494	22.220	1.00	12.56	H	C
ATOM	2531	O	CYS	H	182	31.047	14.379	23.040	1.00	13.75	H	O
ATOM	2532	CB	CYS	H	182	33.605	12.685	22.166	1.00	14.35	H	C
ATOM	2533	SG	CYS	H	182	35.315	12.691	21.563	1.00	16.95	H	S
ATOM	2534	N	ALA	H	183	30.530	12.445	22.005	1.00	10.97	H	N
ATOM	2535	CA	ALA	H	183	29.290	12.254	22.731	1.00	12.15	H	C
ATOM	2536	C	ALA	H	183	28.980	10.769	22.670	1.00	11.48	H	C
ATOM	2537	O	ALA	H	183	29.325	10.102	21.696	1.00	13.04	H	O
ATOM	2538	CB	ALA	H	183	28.166	13.066	22.088	1.00	10.31	H	C
ATOM	2539	N	GLY	H	184A	28.352	10.244	23.714	1.00	11.65	H	N
ATOM	2540	CA	GLY	H	184A	28.016	8.835	23.712	1.00	12.33	H	C
ATOM	2541	C	GLY	H	184A	28.474	8.038	24.916	1.00	13.73	H	C
ATOM	2542	O	GLY	H	184A	28.543	8.545	26.041	1.00	13.45	H	O
ATOM	2543	N	TYR	H	184	28.793	6.773	24.667	1.00	14.78	H	N
ATOM	2544	CA	TYR	H	184	29.217	5.864	25.720	1.00	14.94	H	C
ATOM	2545	C	TYR	H	184	30.395	5.029	25.250	1.00	15.46	H	C
ATOM	2546	O	TYR	H	184	30.509	4.702	24.070	1.00	16.06	H	O
ATOM	2547	CB	TYR	H	184	28.065	4.935	26.112	1.00	16.53	H	C
ATOM	2548	CG	TYR	H	184	26.792	5.637	26.533	1.00	18.74	H	C
ATOM	2549	CD1	TYR	H	184	25.937	6.206	25.589	1.00	18.37	H	C
ATOM	2550	CD2	TYR	H	184	26.443	5.731	27.878	1.00	20.30	H	C
ATOM	2551	CE1	TYR	H	184	24.772	6.847	25.973	1.00	19.02	H	C
ATOM	2552	CE2	TYR	H	184	25.277	6.371	28.273	1.00	19.18	H	C
ATOM	2553	CZ	TYR	H	184	24.448	6.925	27.317	1.00	19.19	H	C
ATOM	2554	OH	TYR	H	184	23.285	7.542	27.699	1.00	21.68	H	O
ATOM	2555	N	SER	H	185	31.267	4.681	26.185	1.00	15.70	H	N
ATOM	2556	CA	SER	H	185	32.450	3.891	25.882	1.00	15.49	H	C
ATOM	2557	C	SER	H	185	32.314	2.426	26.309	1.00	16.42	H	C
ATOM	2558	O	SER	H	185	33.294	1.680	26.293	1.00	16.49	H	O
ATOM	2559	CB	SER	H	185	33.655	4.506	26.579	1.00	15.34	H	C
ATOM	2560	OG	SER	H	185	33.478	4.459	27.984	1.00	15.56	H	O
ATOM	2561	N	ASP	H	186	31.110	2.013	26.691	1.00	17.79	H	N
ATOM	2562	CA	ASP	H	186	30.898	0.633	27.116	1.00	20.64	H	C
ATOM	2563	C	ASP	H	186	30.358	-0.274	26.006	1.00	20.60	H	C
ATOM	2564	O	ASP	H	186	29.934	-1.397	26.268	1.00	20.87	H	O
ATOM	2565	CB	ASP	H	186	29.962	0.589	28.330	1.00	20.43	H	C
ATOM	2566	CG	ASP	H	186	28.576	1.098	28.019	1.00	21.02	H	C
ATOM	2567	OD1	ASP	H	186	28.330	1.483	26.884	1.00	21.60	H	O

ATOM	2568	OD2	ASP	H	186	27.750	1.103	28.921	1.00	21.42	H O
ATOM	2569	N	GLY	H	187	30.373	0.230	24.773	1.00	21.14	H N
ATOM	2570	CA	GLY	H	187	29.914	-0.531	23.625	1.00	20.04	H C
ATOM	2571	C	GLY	H	187	28.424	-0.780	23.493	1.00	21.04	H C
ATOM	2572	O	GLY	H	187	28.022	-1.702	22.789	1.00	22.73	H O
ATOM	2573	N	SER	H	188A	27.597	0.046	24.126	1.00	20.16	H N
ATOM	2574	CA	SER	H	188A	26.153	-0.151	24.068	1.00	18.78	H C
ATOM	2575	C	SER	H	188A	25.337	0.830	23.225	1.00	17.55	H C
ATOM	2576	O	SER	H	188A	24.298	0.457	22.686	1.00	18.92	H O
ATOM	2577	CB	SER	H	188A	25.582	-0.127	25.482	1.00	18.59	H C
ATOM	2578	OG	SER	H	188A	25.675	1.186	26.011	1.00	20.17	H O
ATOM	2579	N	LYS	H	188	25.786	2.076	23.118	1.00	17.33	H N
ATOM	2580	CA	LYS	H	188	25.020	3.091	22.390	1.00	15.93	H C
ATOM	2581	C	LYS	H	188	25.889	4.084	21.610	1.00	15.78	H C
ATOM	2582	O	LYS	H	188	26.883	4.596	22.133	1.00	14.09	H O
ATOM	2583	CB	LYS	H	188	24.140	3.847	23.388	1.00	15.97	H C
ATOM	2584	CG	LYS	H	188	23.127	2.967	24.114	1.00	17.40	H C
ATOM	2585	CD	LYS	H	188	22.386	3.732	25.199	1.00	18.22	H C
ATOM	2586	CE	LYS	H	188	23.253	3.944	26.424	1.00	19.93	H C
ATOM	2587	NZ	LYS	H	188	23.548	2.666	27.142	1.00	23.44	H N
ATOM	2588	N	ASP	H	189	25.487	4.381	20.375	1.00	14.78	H N
ATOM	2589	CA	ASP	H	189	26.254	5.283	19.517	1.00	14.89	H C
ATOM	2590	C	ASP	H	189	25.516	5.427	18.179	1.00	15.27	H C
ATOM	2591	O	ASP	H	189	24.557	4.698	17.911	1.00	12.95	H O
ATOM	2592	CB	ASP	H	189	27.639	4.640	19.305	1.00	15.17	H C
ATOM	2593	CG	ASP	H	189	28.650	5.548	18.606	1.00	14.51	H C
ATOM	2594	OD1	ASP	H	189	28.434	6.750	18.465	1.00	13.62	H O
ATOM	2595	OD2	ASP	H	189	29.685	5.019	18.219	1.00	13.36	H O
ATOM	2596	N	SER	H	190	25.930	6.393	17.363	1.00	12.60	H N
ATOM	2597	CA	SER	H	190	25.358	6.542	16.036	1.00	12.63	H C
ATOM	2598	C	SER	H	190	26.323	5.715	15.176	1.00	14.47	H C
ATOM	2599	O	SER	H	190	27.309	5.184	15.697	1.00	14.59	H O
ATOM	2600	CB	SER	H	190	25.337	8.012	15.595	1.00	12.32	H C
ATOM	2601	OG	SER	H	190	26.590	8.641	15.775	1.00	16.00	H O
ATOM	2602	N	CYS	H	191	26.063	5.592	13.879	1.00	16.70	H N
ATOM	2603	CA	CYS	H	191	26.932	4.786	13.023	1.00	18.01	H C
ATOM	2604	C	CYS	H	191	27.094	5.424	11.651	1.00	18.15	H C
ATOM	2605	O	CYS	H	191	26.502	6.469	11.374	1.00	18.84	H O
ATOM	2606	CB	CYS	H	191	26.336	3.376	12.898	1.00	21.90	H C
ATOM	2607	SG	CYS	H	191	27.470	2.046	12.380	1.00	30.15	H S
ATOM	2608	N	LYS	H	192	27.898	4.791	10.800	1.00	16.09	H N
ATOM	2609	CA	LYS	H	192	28.172	5.271	9.446	1.00	17.53	H C
ATOM	2610	C	LYS	H	192	26.934	5.717	8.668	1.00	15.62	H C
ATOM	2611	O	LYS	H	192	26.914	6.803	8.097	1.00	13.65	H O
ATOM	2612	CB	LYS	H	192	28.898	4.186	8.638	1.00	21.05	H C
ATOM	2613	CG	LYS	H	192	30.199	3.698	9.262	1.00	26.03	H C
ATOM	2614	CD	LYS	H	192	30.964	2.766	8.330	1.00	30.74	H C
ATOM	2615	CE	LYS	H	192	30.199	1.481	8.048	1.00	35.28	H C
ATOM	2616	NZ	LYS	H	192	30.941	0.599	7.093	1.00	36.87	H N
ATOM	2617	N	GLY	H	193	25.910	4.872	8.635	1.00	15.41	H N
ATOM	2618	CA	GLY	H	193	24.698	5.207	7.912	1.00	14.29	H C
ATOM	2619	C	GLY	H	193	23.928	6.392	8.471	1.00	14.66	H C
ATOM	2620	O	GLY	H	193	23.014	6.898	7.822	1.00	13.96	H O
ATOM	2621	N	ASP	H	194	24.287	6.836	9.673	1.00	13.02	H N
ATOM	2622	CA	ASP	H	194	23.627	7.976	10.304	1.00	11.92	H C
ATOM	2623	C	ASP	H	194	24.319	9.299	9.972	1.00	11.87	H C

ATOM	2624	O	ASP	H	194	23.795	10.379	10.273	1.00	10.97	H	O
ATOM	2625	CB	ASP	H	194	23.585	7.780	11.821	1.00	11.34	H	C
ATOM	2626	CG	ASP	H	194	22.824	6.530	12.223	1.00	12.55	H	C
ATOM	2627	OD1	ASP	H	194	21.676	6.411	11.836	1.00	11.16	H	O
ATOM	2628	OD2	ASP	H	194	23.389	5.684	12.923	1.00	10.92	H	O
ATOM	2629	N	SER	H	195	25.492	9.201	9.348	1.00	10.97	H	N
ATOM	2630	CA	SER	H	195	26.290	10.359	8.945	1.00	11.04	H	C
ATOM	2631	C	SER	H	195	25.454	11.500	8.379	1.00	11.57	H	C
ATOM	2632	O	SER	H	195	24.571	11.285	7.545	1.00	10.28	H	O
ATOM	2633	CB	SER	H	195	27.316	9.943	7.890	1.00	9.93	H	C
ATOM	2634	OG	SER	H	195	28.260	9.039	8.425	1.00	14.11	H	O
ATOM	2635	N	GLY	H	196	25.753	12.717	8.824	1.00	12.35	H	N
ATOM	2636	CA	GLY	H	196	25.028	13.884	8.348	1.00	12.23	H	C
ATOM	2637	C	GLY	H	196	23.805	14.182	9.189	1.00	13.45	H	C
ATOM	2638	O	GLY	H	196	23.259	15.286	9.146	1.00	13.77	H	O
ATOM	2639	N	GLY	H	197	23.383	13.187	9.962	1.00	13.04	H	N
ATOM	2640	CA	GLY	H	197	22.222	13.334	10.807	1.00	13.77	H	C
ATOM	2641	C	GLY	H	197	22.427	14.322	11.934	1.00	14.43	H	C
ATOM	2642	O	GLY	H	197	23.558	14.645	12.302	1.00	15.21	H	O
ATOM	2643	N	PRO	H	198	21.327	14.806	12.516	1.00	13.56	H	N
ATOM	2644	CA	PRO	H	198	21.315	15.772	13.615	1.00	13.40	H	C
ATOM	2645	C	PRO	H	198	21.761	15.263	14.981	1.00	11.88	H	C
ATOM	2646	O	PRO	H	198	21.559	14.102	15.330	1.00	11.73	H	O
ATOM	2647	CB	PRO	H	198	19.847	16.220	13.688	1.00	12.32	H	C
ATOM	2648	CG	PRO	H	198	19.183	15.624	12.464	1.00	16.84	H	C
ATOM	2649	CD	PRO	H	198	19.960	14.396	12.164	1.00	14.30	H	C
ATOM	2650	N	HIS	H	199	22.378	16.166	15.730	1.00	10.39	H	N
ATOM	2651	CA	HIS	H	199	22.775	15.954	17.116	1.00	10.13	H	C
ATOM	2652	C	HIS	H	199	22.028	17.189	17.599	1.00	10.86	H	C
ATOM	2653	O	HIS	H	199	22.509	18.312	17.426	1.00	10.19	H	O
ATOM	2654	CB	HIS	H	199	24.284	16.121	17.322	1.00	11.26	H	C
ATOM	2655	CG	HIS	H	199	24.698	16.134	18.765	1.00	9.49	H	C
ATOM	2656	ND1	HIS	H	199	24.605	17.258	19.556	1.00	7.80	H	N
ATOM	2657	CD2	HIS	H	199	25.174	15.151	19.567	1.00	9.62	H	C
ATOM	2658	CE1	HIS	H	199	25.006	16.970	20.782	1.00	9.46	H	C
ATOM	2659	NE2	HIS	H	199	25.356	15.698	20.816	1.00	10.16	H	N
ATOM	2660	N	ALA	H	200	20.826	16.979	18.140	1.00	11.28	H	N
ATOM	2661	CA	ALA	H	200	19.964	18.076	18.578	1.00	11.42	H	C
ATOM	2662	C	ALA	H	200	19.879	18.243	20.085	1.00	10.13	H	C
ATOM	2663	O	ALA	H	200	19.714	17.281	20.819	1.00	8.59	H	O
ATOM	2664	CB	ALA	H	200	18.567	17.893	17.991	1.00	8.70	H	C
ATOM	2665	N	THR	H	201	19.968	19.488	20.531	1.00	10.27	H	N
ATOM	2666	CA	THR	H	201	19.943	19.795	21.950	1.00	11.65	H	C
ATOM	2667	C	THR	H	201	18.690	20.573	22.350	1.00	12.35	H	C
ATOM	2668	O	THR	H	201	18.358	21.590	21.753	1.00	12.80	H	O
ATOM	2669	CB	THR	H	201	21.189	20.616	22.322	1.00	10.77	H	C
ATOM	2670	OG1	THR	H	201	22.354	19.955	21.814	1.00	9.62	H	O
ATOM	2671	CG2	THR	H	201	21.307	20.769	23.823	1.00	5.98	H	C
ATOM	2672	N	HIS	H	202	18.012	20.084	23.379	1.00	12.93	H	N
ATOM	2673	CA	HIS	H	202	16.799	20.709	23.889	1.00	14.16	H	C
ATOM	2674	C	HIS	H	202	17.182	21.718	24.972	1.00	13.17	H	C
ATOM	2675	O	HIS	H	202	17.953	21.406	25.877	1.00	11.26	H	O
ATOM	2676	CB	HIS	H	202	15.883	19.630	24.487	1.00	15.77	H	C
ATOM	2677	CG	HIS	H	202	14.461	20.062	24.661	1.00	19.01	H	C
ATOM	2678	ND1	HIS	H	202	13.551	19.330	25.399	1.00	20.89	H	N
ATOM	2679	CD2	HIS	H	202	13.778	21.124	24.172	1.00	17.67	H	C

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ATOM   2680  CE1 HIS H 202      12.374  19.925  25.356  1.00 18.13      H    C
ATOM   2681  NE2 HIS H 202      12.484  21.016  24.617  1.00 20.03      H    N
ATOM   2682  N   TYR H 203      16.654  22.932  24.878  1.00 13.14      H    N
ATOM   2683  CA  TYR H 203      16.949  23.947  25.882  1.00 14.38      H    C
ATOM   2684  C   TYR H 203      15.762  24.872  26.070  1.00 15.63      H    C
ATOM   2685  O   TYR H 203      15.399  25.617  25.160  1.00 17.55      H    O
ATOM   2686  CB  TYR H 203      18.170  24.788  25.495  1.00 11.34      H    C
ATOM   2687  CG  TYR H 203      18.555  25.767  26.587  1.00 13.03      H    C
ATOM   2688  CD1 TYR H 203      19.202  25.328  27.741  1.00 11.89      H    C
ATOM   2689  CD2 TYR H 203      18.224  27.118  26.494  1.00 11.33      H    C
ATOM   2690  CE1 TYR H 203      19.510  26.208  28.775  1.00 15.40      H    C
ATOM   2691  CE2 TYR H 203      18.520  28.006  27.523  1.00 13.47      H    C
ATOM   2692  CZ  TYR H 203      19.163  27.544  28.660  1.00 15.28      H    C
ATOM   2693  OH  TYR H 203      19.449  28.406  29.689  1.00 17.54      H    O
ATOM   2694  N   ARG H 204      15.162  24.817  27.254  1.00 17.36      H    N
ATOM   2695  CA  ARG H 204      14.019  25.654  27.590  1.00 16.44      H    C
ATOM   2696  C   ARG H 204      12.928  25.702  26.523  1.00 18.12      H    C
ATOM   2697  O   ARG H 204      12.544  26.774  26.054  1.00 19.33      H    O
ATOM   2698  CB  ARG H 204      14.507  27.068  27.931  1.00 18.74      H    C
ATOM   2699  CG  ARG H 204      15.268  27.102  29.256  1.00 21.03      H    C
ATOM   2700  CD  ARG H 204      15.852  28.461  29.633  1.00 23.39      H    C
ATOM   2701  NE  ARG H 204      16.460  28.378  30.965  1.00 29.04      H    N
ATOM   2702  CZ  ARG H 204      17.208  29.320  31.536  1.00 29.55      H    C
ATOM   2703  NH1 ARG H 204      17.473  30.455  30.906  1.00 29.68      H    N
ATOM   2704  NH2 ARG H 204      17.698  29.120  32.753  1.00 30.72      H    N
ATOM   2705  N   GLY H 205      12.437  24.528  26.135  1.00 18.15      H    N
ATOM   2706  CA  GLY H 205      11.366  24.455  25.158  1.00 18.43      H    C
ATOM   2707  C   GLY H 205      11.688  24.465  23.672  1.00 17.94      H    C
ATOM   2708  O   GLY H 205      10.773  24.325  22.859  1.00 20.84      H    O
ATOM   2709  N   THR H 206      12.957  24.613  23.302  1.00 17.15      H    N
ATOM   2710  CA  THR H 206      13.334  24.651  21.889  1.00 16.34      H    C
ATOM   2711  C   THR H 206      14.556  23.786  21.587  1.00 15.73      H    C
ATOM   2712  O   THR H 206      15.485  23.715  22.389  1.00 16.49      H    O
ATOM   2713  CB  THR H 206      13.608  26.111  21.451  1.00 16.85      H    C
ATOM   2714  OG1 THR H 206      12.396  26.859  21.558  1.00 20.04      H    O
ATOM   2715  CG2 THR H 206      14.112  26.181  20.008  1.00 15.79      H    C
ATOM   2716  N   TRP H 207      14.544  23.136  20.424  1.00 14.13      H    N
ATOM   2717  CA  TRP H 207      15.639  22.270  19.995  1.00 11.73      H    C
ATOM   2718  C   TRP H 207      16.582  23.008  19.051  1.00 11.84      H    C
ATOM   2719  O   TRP H 207      16.138  23.745  18.174  1.00 10.36      H    O
ATOM   2720  CB  TRP H 207      15.089  21.025  19.297  1.00 10.05      H    C
ATOM   2721  CG  TRP H 207      14.342  20.115  20.205  1.00 12.23      H    C
ATOM   2722  CD1 TRP H 207      13.032  20.210  20.573  1.00 11.57      H    C
ATOM   2723  CD2 TRP H 207      14.871  18.974  20.891  1.00 12.27      H    C
ATOM   2724  NE1 TRP H 207      12.711  19.197  21.446  1.00 10.79      H    N
ATOM   2725  CE2 TRP H 207      13.821  18.425  21.659  1.00 11.69      H    C
ATOM   2726  CE3 TRP H 207      16.130  18.362  20.927  1.00 10.32      H    C
ATOM   2727  CZ2 TRP H 207      13.994  17.292  22.460  1.00 12.43      H    C
ATOM   2728  CZ3 TRP H 207      16.303  17.233  21.722  1.00 13.70      H    C
ATOM   2729  CH2 TRP H 207      15.239  16.710  22.478  1.00 12.06      H    C
ATOM   2730  N   TYR H 208      17.881  22.785  19.226  1.00 11.22      H    N
ATOM   2731  CA  TYR H 208      18.909  23.446  18.421  1.00 12.37      H    C
ATOM   2732  C   TYR H 208      19.912  22.457  17.832  1.00 12.09      H    C
ATOM   2733  O   TYR H 208      20.175  21.413  18.422  1.00 11.35      H    O
ATOM   2734  CB  TYR H 208      19.679  24.457  19.281  1.00 10.64      H    C
ATOM   2735  CG  TYR H 208      18.818  25.521  19.927  1.00 11.14      H    C
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ATOM	2736	CD1	TYR	H	208	18.192	25.297	21.155	1.00	10.27	H	C
ATOM	2737	CD2	TYR	H	208	18.622	26.756	19.302	1.00	9.96	H	C
ATOM	2738	CE1	TYR	H	208	17.391	26.279	21.746	1.00	9.89	H	C
ATOM	2739	CE2	TYR	H	208	17.823	27.739	19.881	1.00	11.17	H	C
ATOM	2740	CZ	TYR	H	208	17.211	27.496	21.102	1.00	11.59	H	C
ATOM	2741	OH	TYR	H	208	16.417	28.471	21.667	1.00	14.79	H	O
ATOM	2742	N	LEU	H	209	20.479	22.803	16.676	1.00	11.60	H	N
ATOM	2743	CA	LEU	H	209	21.473	21.956	16.019	1.00	10.61	H	C
ATOM	2744	C	LEU	H	209	22.838	22.217	16.655	1.00	11.52	H	C
ATOM	2745	O	LEU	H	209	23.372	23.328	16.572	1.00	9.17	H	O
ATOM	2746	CB	LEU	H	209	21.538	22.275	14.519	1.00	11.62	H	C
ATOM	2747	CG	LEU	H	209	22.533	21.438	13.703	1.00	10.56	H	C
ATOM	2748	CD1	LEU	H	209	22.154	19.964	13.799	1.00	9.75	H	C
ATOM	2749	CD2	LEU	H	209	22.530	21.888	12.253	1.00	11.64	H	C
ATOM	2750	N	THR	H	210	23.401	21.203	17.301	1.00	11.36	H	N
ATOM	2751	CA	THR	H	210	24.703	21.362	17.945	1.00	12.32	H	C
ATOM	2752	C	THR	H	210	25.788	20.487	17.322	1.00	11.28	H	C
ATOM	2753	O	THR	H	210	26.970	20.801	17.411	1.00	11.33	H	O
ATOM	2754	CB	THR	H	210	24.631	21.051	19.464	1.00	11.07	H	C
ATOM	2755	OG1	THR	H	210	23.797	19.907	19.681	1.00	12.24	H	O
ATOM	2756	CG2	THR	H	210	24.069	22.232	20.227	1.00	11.51	H	C
ATOM	2757	N	GLY	H	211	25.392	19.396	16.685	1.00	11.49	H	N
ATOM	2758	CA	GLY	H	211	26.385	18.527	16.085	1.00	12.62	H	C
ATOM	2759	C	GLY	H	211	25.899	17.781	14.861	1.00	12.53	H	C
ATOM	2760	O	GLY	H	211	24.709	17.781	14.540	1.00	10.55	H	O
ATOM	2761	N	ILE	H	212	26.842	17.147	14.174	1.00	12.70	H	N
ATOM	2762	CA	ILE	H	212	26.545	16.371	12.976	1.00	11.37	H	C
ATOM	2763	C	ILE	H	212	27.240	15.016	13.116	1.00	12.64	H	C
ATOM	2764	O	ILE	H	212	28.424	14.961	13.451	1.00	11.86	H	O
ATOM	2765	CB	ILE	H	212	27.094	17.076	11.716	1.00	10.36	H	C
ATOM	2766	CG1	ILE	H	212	26.527	18.498	11.619	1.00	9.87	H	C
ATOM	2767	CG2	ILE	H	212	26.758	16.270	10.485	1.00	7.55	H	C
ATOM	2768	CD1	ILE	H	212	27.194	19.343	10.538	1.00	10.68	H	C
ATOM	2769	N	VAL	H	213	26.503	13.930	12.890	1.00	11.61	H	N
ATOM	2770	CA	VAL	H	213	27.086	12.591	12.969	1.00	10.63	H	C
ATOM	2771	C	VAL	H	213	28.248	12.608	11.976	1.00	10.32	H	C
ATOM	2772	O	VAL	H	213	28.032	12.764	10.773	1.00	10.80	H	O
ATOM	2773	CB	VAL	H	213	26.054	11.512	12.562	1.00	8.77	H	C
ATOM	2774	CG1	VAL	H	213	26.686	10.123	12.627	1.00	7.54	H	C
ATOM	2775	CG2	VAL	H	213	24.850	11.575	13.486	1.00	9.35	H	C
ATOM	2776	N	SER	H	214	29.476	12.465	12.473	1.00	10.48	H	N
ATOM	2777	CA	SER	H	214	30.654	12.533	11.601	1.00	10.02	H	C
ATOM	2778	C	SER	H	214	31.527	11.288	11.510	1.00	10.29	H	C
ATOM	2779	O	SER	H	214	31.662	10.694	10.436	1.00	10.45	H	O
ATOM	2780	CB	SER	H	214	31.525	13.725	12.015	1.00	10.33	H	C
ATOM	2781	OG	SER	H	214	32.650	13.856	11.156	1.00	14.56	H	O
ATOM	2782	N	TRP	H	215	32.144	10.894	12.616	1.00	9.38	H	N
ATOM	2783	CA	TRP	H	215	32.996	9.715	12.571	1.00	9.84	H	C
ATOM	2784	C	TRP	H	215	33.186	9.044	13.919	1.00	11.40	H	C
ATOM	2785	O	TRP	H	215	32.595	9.440	14.925	1.00	10.83	H	O
ATOM	2786	CB	TRP	H	215	34.372	10.077	11.979	1.00	11.73	H	C
ATOM	2787	CG	TRP	H	215	35.189	11.045	12.802	1.00	11.28	H	C
ATOM	2788	CD1	TRP	H	215	35.054	12.405	12.851	1.00	12.73	H	C
ATOM	2789	CD2	TRP	H	215	36.286	10.720	13.670	1.00	12.20	H	C
ATOM	2790	NE1	TRP	H	215	36.002	12.949	13.690	1.00	12.73	H	N
ATOM	2791	CE2	TRP	H	215	36.770	11.937	14.206	1.00	13.66	H	C

ATOM	2792	CE3	TRP	H	215	36.907	9.520	14.044	1.00	11.80	H C
ATOM	2793	CZ2	TRP	H	215	37.852	11.986	15.100	1.00	11.52	H C
ATOM	2794	CZ3	TRP	H	215	37.986	9.569	14.936	1.00	11.59	H C
ATOM	2795	CH2	TRP	H	215	38.445	10.796	15.451	1.00	12.21	H C
ATOM	2796	N	GLY	H	216	34.029	8.020	13.928	1.00	12.15	H N
ATOM	2797	CA	GLY	H	216	34.308	7.298	15.151	1.00	14.20	H C
ATOM	2798	C	GLY	H	216	34.988	6.002	14.792	1.00	15.73	H C
ATOM	2799	O	GLY	H	216	35.124	5.684	13.611	1.00	17.05	H O
ATOM	2800	N	GLN	H	217	35.435	5.255	15.792	1.00	17.07	H N
ATOM	2801	CA	GLN	H	217	36.081	3.982	15.521	1.00	19.04	H C
ATOM	2802	C	GLN	H	217	34.986	2.937	15.544	1.00	17.72	H C
ATOM	2803	O	GLN	H	217	34.486	2.579	16.606	1.00	19.73	H O
ATOM	2804	CB	GLN	H	217	37.136	3.683	16.579	1.00	22.69	H C
ATOM	2805	CG	GLN	H	217	37.813	2.342	16.395	1.00	27.55	H C
ATOM	2806	CD	GLN	H	217	39.254	2.360	16.845	1.00	33.39	H C
ATOM	2807	OE1	GLN	H	217	39.613	3.063	17.791	1.00	34.21	H O
ATOM	2808	NE2	GLN	H	217	40.092	1.576	16.173	1.00	37.35	H N
ATOM	2809	N	GLY	H	219	34.606	2.458	14.364	1.00	18.12	H N
ATOM	2810	CA	GLY	H	219	33.539	1.482	14.279	1.00	17.60	H C
ATOM	2811	C	GLY	H	219	32.283	2.125	14.835	1.00	20.54	H C
ATOM	2812	O	GLY	H	219	32.135	3.347	14.788	1.00	20.64	H O
ATOM	2813	N	CYS	H	220	31.381	1.311	15.372	1.00	21.24	H N
ATOM	2814	CA	CYS	H	220	30.145	1.824	15.943	1.00	23.06	H C
ATOM	2815	C	CYS	H	220	29.893	1.193	17.310	1.00	22.01	H C
ATOM	2816	O	CYS	H	220	29.765	-0.028	17.432	1.00	22.87	H O
ATOM	2817	CB	CYS	H	220	28.981	1.549	14.983	1.00	23.60	H C
ATOM	2818	SG	CYS	H	220	29.194	2.422	13.398	1.00	28.32	H S
ATOM	2819	N	ALA	H	221A	29.830	2.039	18.333	1.00	21.07	H N
ATOM	2820	CA	ALA	H	221A	29.613	1.586	19.704	1.00	21.19	H C
ATOM	2821	C	ALA	H	221A	30.719	0.615	20.102	1.00	20.46	H C
ATOM	2822	O	ALA	H	221A	30.463	-0.454	20.660	1.00	21.19	H O
ATOM	2823	CB	ALA	H	221A	28.245	0.916	19.833	1.00	20.81	H C
ATOM	2824	N	THR	H	221	31.953	0.992	19.797	1.00	20.10	H N
ATOM	2825	CA	THR	H	221	33.109	0.173	20.121	1.00	19.79	H C
ATOM	2826	C	THR	H	221	33.530	0.484	21.551	1.00	18.64	H C
ATOM	2827	O	THR	H	221	33.610	1.647	21.943	1.00	17.97	H O
ATOM	2828	CB	THR	H	221	34.273	0.467	19.151	1.00	20.35	H C
ATOM	2829	OG1	THR	H	221	33.854	0.169	17.815	1.00	22.66	H O
ATOM	2830	CG2	THR	H	221	35.492	-0.386	19.485	1.00	22.20	H C
ATOM	2831	N	VAL	H	222	33.776	-0.560	22.332	1.00	16.93	H N
ATOM	2832	CA	VAL	H	222	34.186	-0.402	23.721	1.00	16.22	H C
ATOM	2833	C	VAL	H	222	35.458	0.437	23.788	1.00	16.60	H C
ATOM	2834	O	VAL	H	222	36.424	0.173	23.077	1.00	16.78	H O
ATOM	2835	CB	VAL	H	222	34.444	-1.783	24.388	1.00	15.57	H C
ATOM	2836	CG1	VAL	H	222	34.994	-1.596	25.802	1.00	15.54	H C
ATOM	2837	CG2	VAL	H	222	33.147	-2.589	24.433	1.00	12.31	H C
ATOM	2838	N	GLY	H	223	35.444	1.458	24.639	1.00	18.10	H N
ATOM	2839	CA	GLY	H	223	36.603	2.322	24.785	1.00	17.10	H C
ATOM	2840	C	GLY	H	223	36.607	3.503	23.834	1.00	16.65	H C
ATOM	2841	O	GLY	H	223	37.602	4.221	23.749	1.00	16.09	H O
ATOM	2842	N	HIS	H	224	35.501	3.716	23.122	1.00	14.21	H N
ATOM	2843	CA	HIS	H	224	35.418	4.817	22.172	1.00	14.13	H C
ATOM	2844	C	HIS	H	224	34.054	5.490	22.169	1.00	13.03	H C
ATOM	2845	O	HIS	H	224	33.043	4.883	22.523	1.00	12.79	H O
ATOM	2846	CB	HIS	H	224	35.772	4.324	20.768	1.00	14.15	H C
ATOM	2847	CG	HIS	H	224	37.163	3.786	20.665	1.00	18.68	H C

ATOM	2848	ND1	HIS	H	224	38.273	4.602	20.632	1.00	22.89	H N
ATOM	2849	CD2	HIS	H	224	37.630	2.516	20.690	1.00	18.87	H C
ATOM	2850	CE1	HIS	H	224	39.365	3.859	20.645	1.00	20.95	H C
ATOM	2851	NE2	HIS	H	224	39.002	2.590	20.682	1.00	24.07	H N
ATOM	2852	N	PHE	H	225	34.059	6.758	21.772	1.00	12.58	H N
ATOM	2853	CA	PHE	H	225	32.870	7.597	21.709	1.00	13.20	H C
ATOM	2854	C	PHE	H	225	32.638	8.059	20.270	1.00	14.27	H C
ATOM	2855	O	PHE	H	225	33.567	8.102	19.459	1.00	13.13	H O
ATOM	2856	CB	PHE	H	225	33.070	8.857	22.566	1.00	12.36	H C
ATOM	2857	CG	PHE	H	225	33.176	8.599	24.041	1.00	13.26	H C
ATOM	2858	CD1	PHE	H	225	32.034	8.486	24.826	1.00	10.55	H C
ATOM	2859	CD2	PHE	H	225	34.422	8.496	24.655	1.00	12.18	H C
ATOM	2860	CE1	PHE	H	225	32.132	8.275	26.197	1.00	11.54	H C
ATOM	2861	CE2	PHE	H	225	34.528	8.284	26.024	1.00	11.28	H C
ATOM	2862	CZ	PHE	H	225	33.383	8.173	26.797	1.00	11.86	H C
ATOM	2863	N	GLY	H	226	31.401	8.423	19.954	1.00	11.84	H N
ATOM	2864	CA	GLY	H	226	31.141	8.930	18.622	1.00	11.14	H C
ATOM	2865	C	GLY	H	226	31.706	10.345	18.564	1.00	11.37	H C
ATOM	2866	O	GLY	H	226	31.783	11.018	19.593	1.00	9.76	H O
ATOM	2867	N	VAL	H	227	32.124	10.789	17.383	1.00	10.30	H N
ATOM	2868	CA	VAL	H	227	32.664	12.137	17.217	1.00	11.99	H C
ATOM	2869	C	VAL	H	227	31.711	12.893	16.279	1.00	12.30	H C
ATOM	2870	O	VAL	H	227	31.308	12.376	15.236	1.00	11.88	H O
ATOM	2871	CB	VAL	H	227	34.096	12.119	16.597	1.00	13.42	H C
ATOM	2872	CG1	VAL	H	227	34.725	13.503	16.711	1.00	10.66	H C
ATOM	2873	CG2	VAL	H	227	34.977	11.081	17.304	1.00	11.39	H C
ATOM	2874	N	TYR	H	228	31.360	14.117	16.651	1.00	11.76	H N
ATOM	2875	CA	TYR	H	228	30.424	14.913	15.868	1.00	11.60	H C
ATOM	2876	C	TYR	H	228	31.040	16.251	15.458	1.00	11.78	H C
ATOM	2877	O	TYR	H	228	31.870	16.798	16.176	1.00	12.87	H O
ATOM	2878	CB	TYR	H	228	29.147	15.158	16.692	1.00	12.02	H C
ATOM	2879	CG	TYR	H	228	28.446	13.883	17.159	1.00	13.58	H C
ATOM	2880	CD1	TYR	H	228	28.956	13.112	18.211	1.00	15.38	H C
ATOM	2881	CD2	TYR	H	228	27.302	13.425	16.515	1.00	12.87	H C
ATOM	2882	CE1	TYR	H	228	28.334	11.908	18.599	1.00	13.68	H C
ATOM	2883	CE2	TYR	H	228	26.680	12.235	16.894	1.00	11.86	H C
ATOM	2884	CZ	TYR	H	228	27.198	11.484	17.931	1.00	13.33	H C
ATOM	2885	OH	TYR	H	228	26.570	10.310	18.293	1.00	13.39	H O
ATOM	2886	N	THR	H	229	30.649	16.767	14.296	1.00	10.21	H N
ATOM	2887	CA	THR	H	229	31.158	18.056	13.840	1.00	9.23	H C
ATOM	2888	C	THR	H	229	30.612	19.105	14.817	1.00	9.22	H C
ATOM	2889	O	THR	H	229	29.422	19.093	15.133	1.00	9.33	H O
ATOM	2890	CB	THR	H	229	30.656	18.383	12.420	1.00	11.04	H C
ATOM	2891	OG1	THR	H	229	31.037	17.334	11.519	1.00	10.26	H O
ATOM	2892	CG2	THR	H	229	31.246	19.712	11.935	1.00	8.87	H C
ATOM	2893	N	ARG	H	230	31.473	19.993	15.309	1.00	7.76	H N
ATOM	2894	CA	ARG	H	230	31.051	21.026	16.257	1.00	7.07	H C
ATOM	2895	C	ARG	H	230	30.444	22.197	15.487	1.00	7.98	H C
ATOM	2896	O	ARG	H	230	31.150	23.158	15.134	1.00	6.49	H O
ATOM	2897	CB	ARG	H	230	32.251	21.505	17.093	1.00	8.54	H C
ATOM	2898	CG	ARG	H	230	31.885	22.461	18.238	1.00	11.66	H C
ATOM	2899	CD	ARG	H	230	33.104	22.903	19.054	1.00	14.39	H C
ATOM	2900	NE	ARG	H	230	33.846	21.777	19.631	1.00	14.90	H N
ATOM	2901	CZ	ARG	H	230	33.986	21.545	20.937	1.00	19.51	H C
ATOM	2902	NH1	ARG	H	230	33.434	22.355	21.835	1.00	18.42	H N
ATOM	2903	NH2	ARG	H	230	34.694	20.503	21.356	1.00	18.54	H N

ATOM	2904	N	VAL	H	231	29.134	22.115	15.243	1.00	7.40	H	N
ATOM	2905	CA	VAL	H	231	28.396	23.132	14.485	1.00	8.02	H	C
ATOM	2906	C	VAL	H	231	28.582	24.590	14.906	1.00	8.03	H	C
ATOM	2907	O	VAL	H	231	28.522	25.478	14.063	1.00	11.15	H	O
ATOM	2908	CB	VAL	H	231	26.869	22.813	14.453	1.00	8.34	H	C
ATOM	2909	CG1	VAL	H	231	26.091	23.963	13.789	1.00	6.76	H	C
ATOM	2910	CG2	VAL	H	231	26.631	21.536	13.663	1.00	6.77	H	C
ATOM	2911	N	SER	H	232	28.812	24.846	16.191	1.00	9.98	H	N
ATOM	2912	CA	SER	H	232	28.999	26.216	16.665	1.00	10.61	H	C
ATOM	2913	C	SER	H	232	30.141	26.942	15.951	1.00	11.51	H	C
ATOM	2914	O	SER	H	232	30.116	28.162	15.815	1.00	13.83	H	O
ATOM	2915	CB	SER	H	232	29.253	26.225	18.172	1.00	9.74	H	C
ATOM	2916	OG	SER	H	232	30.328	25.366	18.508	1.00	9.99	H	O
ATOM	2917	N	GLN	H	233	31.138	26.192	15.500	1.00	10.91	H	N
ATOM	2918	CA	GLN	H	233	32.282	26.758	14.790	1.00	12.68	H	C
ATOM	2919	C	GLN	H	233	31.957	27.212	13.365	1.00	12.56	H	C
ATOM	2920	O	GLN	H	233	32.715	27.973	12.755	1.00	10.39	H	O
ATOM	2921	CB	GLN	H	233	33.410	25.725	14.738	1.00	14.26	H	C
ATOM	2922	CG	GLN	H	233	33.859	25.290	16.109	1.00	17.78	H	C
ATOM	2923	CD	GLN	H	233	34.180	26.481	16.983	1.00	23.92	H	C
ATOM	2924	OE1	GLN	H	233	35.120	27.221	16.702	1.00	22.25	H	O
ATOM	2925	NE2	GLN	H	233	33.383	26.687	18.045	1.00	25.97	H	N
ATOM	2926	N	TYR	H	234	30.815	26.765	12.851	1.00	10.53	H	N
ATOM	2927	CA	TYR	H	234	30.401	27.072	11.485	1.00	10.91	H	C
ATOM	2928	C	TYR	H	234	29.164	27.970	11.338	1.00	11.10	H	C
ATOM	2929	O	TYR	H	234	28.663	28.137	10.232	1.00	12.26	H	O
ATOM	2930	CB	TYR	H	234	30.145	25.748	10.752	1.00	11.97	H	C
ATOM	2931	CG	TYR	H	234	31.359	24.833	10.717	1.00	10.28	H	C
ATOM	2932	CD1	TYR	H	234	32.363	25.018	9.765	1.00	9.58	H	C
ATOM	2933	CD2	TYR	H	234	31.526	23.826	11.661	1.00	8.26	H	C
ATOM	2934	CE1	TYR	H	234	33.501	24.231	9.756	1.00	10.13	H	C
ATOM	2935	CE2	TYR	H	234	32.673	23.022	11.665	1.00	10.83	H	C
ATOM	2936	CZ	TYR	H	234	33.653	23.236	10.707	1.00	10.93	H	C
ATOM	2937	OH	TYR	H	234	34.782	22.464	10.691	1.00	11.60	H	O
ATOM	2938	N	ILE	H	235	28.670	28.549	12.428	1.00	10.49	H	N
ATOM	2939	CA	ILE	H	235	27.473	29.389	12.341	1.00	12.21	H	C
ATOM	2940	C	ILE	H	235	27.624	30.539	11.343	1.00	13.01	H	C
ATOM	2941	O	ILE	H	235	26.790	30.710	10.455	1.00	13.67	H	O
ATOM	2942	CB	ILE	H	235	27.076	29.971	13.725	1.00	12.39	H	C
ATOM	2943	CG1	ILE	H	235	26.910	28.842	14.746	1.00	13.92	H	C
ATOM	2944	CG2	ILE	H	235	25.759	30.764	13.601	1.00	14.14	H	C
ATOM	2945	CD1	ILE	H	235	25.923	27.750	14.319	1.00	11.48	H	C
ATOM	2946	N	GLU	H	236	28.680	31.331	11.493	1.00	15.53	H	N
ATOM	2947	CA	GLU	H	236	28.931	32.449	10.582	1.00	16.27	H	C
ATOM	2948	C	GLU	H	236	29.116	31.967	9.143	1.00	15.01	H	C
ATOM	2949	O	GLU	H	236	28.608	32.575	8.199	1.00	15.26	H	O
ATOM	2950	CB	GLU	H	236	30.178	33.222	11.023	1.00	20.86	H	C
ATOM	2951	CG	GLU	H	236	30.002	34.066	12.278	1.00	28.52	H	C
ATOM	2952	CD	GLU	H	236	29.769	33.243	13.535	1.00	35.96	H	C
ATOM	2953	OE1	GLU	H	236	30.614	32.384	13.848	1.00	39.48	H	O
ATOM	2954	OE2	GLU	H	236	28.742	33.466	14.205	1.00	39.32	H	O
ATOM	2955	N	TRP	H	237	29.848	30.873	8.979	1.00	13.41	H	N
ATOM	2956	CA	TRP	H	237	30.098	30.298	7.660	1.00	12.55	H	C
ATOM	2957	C	TRP	H	237	28.759	29.950	7.000	1.00	13.34	H	C
ATOM	2958	O	TRP	H	237	28.524	30.268	5.828	1.00	12.48	H	O
ATOM	2959	CB	TRP	H	237	30.950	29.023	7.807	1.00	12.29	H	C

ATOM	2960	CG	TRP	H	237	31.424	28.400	6.509	1.00	10.83	H C
ATOM	2961	CD1	TRP	H	237	32.421	28.860	5.690	1.00	11.49	H C
ATOM	2962	CD2	TRP	H	237	30.927	27.196	5.897	1.00	11.56	H C
ATOM	2963	NE1	TRP	H	237	32.577	28.019	4.612	1.00	11.23	H N
ATOM	2964	CE2	TRP	H	237	31.675	26.993	4.711	1.00	10.61	H C
ATOM	2965	CE3	TRP	H	237	29.922	26.276	6.232	1.00	11.81	H C
ATOM	2966	CZ2	TRP	H	237	31.448	25.903	3.856	1.00	10.86	H C
ATOM	2967	CZ3	TRP	H	237	29.695	25.186	5.379	1.00	13.69	H C
ATOM	2968	CH2	TRP	H	237	30.459	25.013	4.202	1.00	11.69	H C
ATOM	2969	N	LEU	H	238	27.890	29.289	7.762	1.00	11.93	H N
ATOM	2970	CA	LEU	H	238	26.577	28.876	7.272	1.00	13.74	H C
ATOM	2971	C	LEU	H	238	25.660	30.064	6.976	1.00	14.26	H C
ATOM	2972	O	LEU	H	238	25.006	30.106	5.937	1.00	15.47	H O
ATOM	2973	CB	LEU	H	238	25.906	27.948	8.296	1.00	11.48	H C
ATOM	2974	CG	LEU	H	238	26.619	26.607	8.530	1.00	12.33	H C
ATOM	2975	CD1	LEU	H	238	26.127	25.955	9.816	1.00	9.88	H C
ATOM	2976	CD2	LEU	H	238	26.393	25.696	7.330	1.00	11.54	H C
ATOM	2977	N	GLN	H	239	25.614	31.029	7.887	1.00	16.12	H N
ATOM	2978	CA	GLN	H	239	24.761	32.202	7.696	1.00	18.31	H C
ATOM	2979	C	GLN	H	239	25.149	33.011	6.463	1.00	17.63	H C
ATOM	2980	O	GLN	H	239	24.289	33.448	5.705	1.00	17.31	H O
ATOM	2981	CB	GLN	H	239	24.809	33.099	8.930	1.00	16.56	H C
ATOM	2982	CG	GLN	H	239	24.263	32.442	10.176	1.00	22.50	H C
ATOM	2983	CD	GLN	H	239	24.217	33.393	11.348	1.00	24.81	H C
ATOM	2984	OE1	GLN	H	239	25.143	34.179	11.563	1.00	28.05	H O
ATOM	2985	NE2	GLN	H	239	23.144	33.321	12.124	1.00	28.34	H N
ATOM	2986	N	LYS	H	240	26.446	33.205	6.268	1.00	19.23	H N
ATOM	2987	CA	LYS	H	240	26.944	33.958	5.125	1.00	20.76	H C
ATOM	2988	C	LYS	H	240	26.544	33.269	3.816	1.00	20.55	H C
ATOM	2989	O	LYS	H	240	26.068	33.915	2.884	1.00	20.97	H O
ATOM	2990	CB	LYS	H	240	28.467	34.072	5.218	1.00	23.48	H C
ATOM	2991	CG	LYS	H	240	29.082	35.190	4.391	1.00	30.47	H C
ATOM	2992	CD	LYS	H	240	29.016	34.913	2.900	1.00	34.65	H C
ATOM	2993	CE	LYS	H	240	29.606	36.071	2.101	1.00	38.36	H C
ATOM	2994	NZ	LYS	H	240	31.028	36.326	2.469	1.00	39.99	H N
ATOM	2995	N	LEU	H	241	26.733	31.954	3.754	1.00	20.03	H N
ATOM	2996	CA	LEU	H	241	26.398	31.187	2.560	1.00	19.49	H C
ATOM	2997	C	LEU	H	241	24.900	31.140	2.256	1.00	19.86	H C
ATOM	2998	O	LEU	H	241	24.508	31.126	1.094	1.00	18.70	H O
ATOM	2999	CB	LEU	H	241	26.948	29.763	2.680	1.00	19.02	H C
ATOM	3000	CG	LEU	H	241	28.473	29.630	2.647	1.00	19.62	H C
ATOM	3001	CD1	LEU	H	241	28.870	28.191	2.990	1.00	18.89	H C
ATOM	3002	CD2	LEU	H	241	29.001	30.032	1.273	1.00	14.59	H C
ATOM	3003	N	MET	H	242	24.058	31.106	3.287	1.00	21.92	H N
ATOM	3004	CA	MET	H	242	22.615	31.081	3.051	1.00	24.59	H C
ATOM	3005	C	MET	H	242	22.142	32.421	2.477	1.00	27.60	H C
ATOM	3006	O	MET	H	242	21.097	32.497	1.834	1.00	27.62	H O
ATOM	3007	CB	MET	H	242	21.854	30.746	4.341	1.00	21.21	H C
ATOM	3008	CG	MET	H	242	22.003	29.283	4.768	1.00	20.37	H C
ATOM	3009	SD	MET	H	242	21.011	28.815	6.206	1.00	18.95	H S
ATOM	3010	CE	MET	H	242	21.948	29.603	7.540	1.00	14.65	H C
ATOM	3011	N	ARG	H	243	22.924	33.472	2.703	1.00	30.45	H N
ATOM	3012	CA	ARG	H	243	22.595	34.795	2.187	1.00	34.75	H C
ATOM	3013	C	ARG	H	243	23.270	35.048	0.840	1.00	37.34	H C
ATOM	3014	O	ARG	H	243	23.277	36.176	0.351	1.00	39.24	H O
ATOM	3015	CB	ARG	H	243	23.048	35.868	3.170	1.00	35.66	H C

ATOM	3016	CG	ARG	H	243	22.216	35.976	4.429	1.00	37.59	H C
ATOM	3017	CD	ARG	H	243	23.094	36.381	5.600	1.00	42.39	H C
ATOM	3018	NE	ARG	H	243	24.090	37.380	5.218	1.00	45.18	H N
ATOM	3019	CZ	ARG	H	243	25.137	37.722	5.965	1.00	46.96	H C
ATOM	3020	NH1	ARG	H	243	25.335	37.148	7.147	1.00	45.77	H N
ATOM	3021	NH2	ARG	H	243	25.997	38.631	5.519	1.00	47.07	H N
ATOM	3022	N	SER	H	244	23.836	34.002	0.245	1.00	39.09	H N
ATOM	3023	CA	SER	H	244	24.522	34.130	-1.034	1.00	40.99	H C
ATOM	3024	C	SER	H	244	23.684	33.644	-2.208	1.00	42.62	H C
ATOM	3025	O	SER	H	244	22.743	32.867	-2.042	1.00	41.83	H O
ATOM	3026	CB	SER	H	244	25.845	33.363	-0.994	1.00	41.34	H C
ATOM	3027	OG	SER	H	244	26.705	33.895	-0.001	1.00	43.40	H O
ATOM	3028	N	GLU	H	245	24.038	34.113	-3.400	1.00	44.75	H N
ATOM	3029	CA	GLU	H	245	23.330	33.737	-4.615	1.00	46.58	H C
ATOM	3030	C	GLU	H	245	23.882	32.431	-5.165	1.00	46.31	H C
ATOM	3031	O	GLU	H	245	25.076	32.157	-5.057	1.00	46.57	H O
ATOM	3032	CB	GLU	H	245	23.470	34.833	-5.672	1.00	49.32	H C
ATOM	3033	CG	GLU	H	245	22.851	36.164	-5.282	1.00	53.68	H C
ATOM	3034	CD	GLU	H	245	22.994	37.212	-6.369	1.00	56.49	H C
ATOM	3035	OE1	GLU	H	245	22.529	38.339	-6.166	1.00	58.31	H O
ATOM	3036	OE2	GLU	H	245	23.571	36.900	-7.417	1.00	57.52	H O
ATOM	3037	N	PRO	H	246	23.013	31.605	-5.765	1.00	46.06	H N
ATOM	3038	CA	PRO	H	246	23.430	30.323	-6.334	1.00	46.49	H C
ATOM	3039	C	PRO	H	246	24.612	30.488	-7.287	1.00	46.82	H C
ATOM	3040	O	PRO	H	246	24.884	31.588	-7.770	1.00	47.98	H O
ATOM	3041	CB	PRO	H	246	22.174	29.846	-7.055	1.00	46.60	H C
ATOM	3042	CG	PRO	H	246	21.081	30.401	-6.206	1.00	46.59	H C
ATOM	3043	CD	PRO	H	246	21.563	31.803	-5.932	1.00	45.49	H C
ATOM	3044	N	ARG	H	247	25.316	29.393	-7.545	1.00	45.68	H N
ATOM	3045	CA	ARG	H	247	26.455	29.420	-8.449	1.00	45.13	H C
ATOM	3046	C	ARG	H	247	26.391	28.204	-9.360	1.00	43.90	H C
ATOM	3047	O	ARG	H	247	26.012	27.114	-8.930	1.00	43.91	H O
ATOM	3048	CB	ARG	H	247	27.772	29.416	-7.665	1.00	46.78	H C
ATOM	3049	CG	ARG	H	247	27.999	30.655	-6.806	1.00	48.61	H C
ATOM	3050	CD	ARG	H	247	29.351	30.585	-6.107	1.00	50.94	H C
ATOM	3051	NE	ARG	H	247	29.547	31.650	-5.121	1.00	52.94	H N
ATOM	3052	CZ	ARG	H	247	28.897	31.748	-3.962	1.00	53.90	H C
ATOM	3053	NH1	ARG	H	247	27.988	30.846	-3.611	1.00	53.30	H N
ATOM	3054	NH2	ARG	H	247	29.164	32.756	-3.142	1.00	54.90	H N
ATOM	3055	N	PRO	H	248	26.754	28.378	-10.639	1.00	42.02	H N
ATOM	3056	CA	PRO	H	248	26.725	27.268	-11.595	1.00	40.10	H C
ATOM	3057	C	PRO	H	248	27.396	26.040	-10.999	1.00	36.76	H C
ATOM	3058	O	PRO	H	248	28.348	26.168	-10.238	1.00	37.56	H O
ATOM	3059	CB	PRO	H	248	27.495	27.826	-12.786	1.00	40.68	H C
ATOM	3060	CG	PRO	H	248	27.146	29.282	-12.741	1.00	43.23	H C
ATOM	3061	CD	PRO	H	248	27.282	29.600	-11.269	1.00	41.68	H C
ATOM	3062	N	GLY	H	249	26.897	24.858	-11.341	1.00	33.94	H N
ATOM	3063	CA	GLY	H	249	27.483	23.636	-10.818	1.00	30.93	H C
ATOM	3064	C	GLY	H	249	27.004	23.304	-9.416	1.00	27.97	H C
ATOM	3065	O	GLY	H	249	26.983	24.164	-8.536	1.00	28.75	H O
ATOM	3066	N	VAL	H	250	26.627	22.047	-9.210	1.00	25.90	H N
ATOM	3067	CA	VAL	H	250	26.137	21.584	-7.916	1.00	22.51	H C
ATOM	3068	C	VAL	H	250	27.154	21.751	-6.785	1.00	20.73	H C
ATOM	3069	O	VAL	H	250	26.866	22.406	-5.783	1.00	19.56	H O
ATOM	3070	CB	VAL	H	250	25.708	20.091	-7.989	1.00	22.46	H C
ATOM	3071	CG1	VAL	H	250	25.243	19.603	-6.616	1.00	21.14	H C

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ATOM   3072  CG2 VAL H 250      24.588  19.924  -9.000  1.00 22.82      H    C
ATOM   3073  N   LEU H 251      28.337  21.165  -6.950  1.00 18.48      H    N
ATOM   3074  CA  LEU H 251      29.380  21.230  -5.929  1.00 18.83      H    C
ATOM   3075  C   LEU H 251      30.070  22.588  -5.808  1.00 19.13      H    C
ATOM   3076  O   LEU H 251      30.520  23.164  -6.790  1.00 18.06      H    O
ATOM   3077  CB  LEU H 251      30.431  20.146  -6.192  1.00 16.90      H    C
ATOM   3078  CG  LEU H 251      31.581  20.002  -5.186  1.00 17.64      H    C
ATOM   3079  CD1 LEU H 251      31.029  19.732  -3.787  1.00 15.90      H    C
ATOM   3080  CD2 LEU H 251      32.504  18.862  -5.628  1.00 16.46      H    C
ATOM   3081  N   LEU H 252      30.151  23.096  -4.586  1.00 19.09      H    N
ATOM   3082  CA  LEU H 252      30.808  24.369  -4.342  1.00 18.91      H    C
ATOM   3083  C   LEU H 252      31.699  24.284  -3.109  1.00 19.51      H    C
ATOM   3084  O   LEU H 252      31.261  23.835  -2.054  1.00 20.23      H    O
ATOM   3085  CB  LEU H 252      29.777  25.476  -4.129  1.00 19.71      H    C
ATOM   3086  CG  LEU H 252      30.362  26.831  -3.726  1.00 21.00      H    C
ATOM   3087  CD1 LEU H 252      31.252  27.360  -4.845  1.00 21.46      H    C
ATOM   3088  CD2 LEU H 252      29.237  27.808  -3.431  1.00 21.39      H    C
ATOM   3089  N   ARG H 253      32.951  24.703  -3.247  1.00 17.62      H    N
ATOM   3090  CA  ARG H 253      33.869  24.704  -2.119  1.00 17.97      H    C
ATOM   3091  C   ARG H 253      34.015  26.150  -1.688  1.00 17.05      H    C
ATOM   3092  O   ARG H 253      34.559  26.970  -2.426  1.00 15.25      H    O
ATOM   3093  CB  ARG H 253      35.230  24.123  -2.511  1.00 18.44      H    C
ATOM   3094  CG  ARG H 253      35.358  22.635  -2.232  1.00 20.42      H    C
ATOM   3095  CD  ARG H 253      34.282  21.846  -2.952  1.00 21.21      H    C
ATOM   3096  NE  ARG H 253      34.476  21.856  -4.397  1.00 21.18      H    N
ATOM   3097  CZ  ARG H 253      35.307  21.047  -5.047  1.00 22.46      H    C
ATOM   3098  NH1 ARG H 253      36.028  20.152  -4.380  1.00 23.51      H    N
ATOM   3099  NH2 ARG H 253      35.414  21.126  -6.367  1.00 19.08      H    N
ATOM   3100  N   ALA H 254      33.499  26.458  -0.501  1.00 16.11      H    N
ATOM   3101  CA  ALA H 254      33.542  27.815   0.028  1.00 15.47      H    C
ATOM   3102  C   ALA H 254      34.658  27.919   1.047  1.00 16.28      H    C
ATOM   3103  O   ALA H 254      34.879  27.003   1.843  1.00 15.62      H    O
ATOM   3104  CB  ALA H 254      32.205  28.179   0.664  1.00 13.69      H    C
ATOM   3105  N   PRO H 255      35.381  29.044   1.039  1.00 15.40      H    N
ATOM   3106  CA  PRO H 255      36.475  29.191   1.994  1.00 14.78      H    C
ATOM   3107  C   PRO H 255      36.048  29.162   3.445  1.00 14.38      H    C
ATOM   3108  O   PRO H 255      34.935  29.556   3.798  1.00 13.71      H    O
ATOM   3109  CB  PRO H 255      37.116  30.526   1.594  1.00 15.88      H    C
ATOM   3110  CG  PRO H 255      35.987  31.294   0.995  1.00 15.99      H    C
ATOM   3111  CD  PRO H 255      35.233  30.249   0.200  1.00 16.40      H    C
ATOM   3112  N   PHE H 256      36.943  28.663   4.281  1.00 13.80      H    N
ATOM   3113  CA  PHE H 256      36.701  28.616   5.706  1.00 16.87      H    C
ATOM   3114  C   PHE H 256      38.005  28.945   6.408  1.00 17.50      H    C
ATOM   3115  O   PHE H 256      39.049  28.394   6.067  1.00 18.45      H    O
ATOM   3116  CB  PHE H 256      36.243  27.240   6.174  1.00 14.38      H    C
ATOM   3117  CG  PHE H 256      35.955  27.201   7.641  1.00 16.91      H    C
ATOM   3118  CD1 PHE H 256      34.773  27.744   8.141  1.00 16.40      H    C
ATOM   3119  CD2 PHE H 256      36.909  26.729   8.538  1.00 16.52      H    C
ATOM   3120  CE1 PHE H 256      34.546  27.828   9.509  1.00 17.72      H    C
ATOM   3121  CE2 PHE H 256      36.692  26.809   9.911  1.00 17.93      H    C
ATOM   3122  CZ  PHE H 256      35.510  27.362  10.398  1.00 18.72      H    C
ATOM   3123  N   PRO H 257      37.960  29.830   7.413  1.00 18.95      H    N
ATOM   3124  CA  PRO H 257      36.765  30.512   7.921  1.00 20.37      H    C
ATOM   3125  C   PRO H 257      36.095  31.426   6.893  1.00 22.86      H    C
ATOM   3126  O   PRO H 257      34.888  31.666   7.011  1.00 23.60      H    O
ATOM   3127  CB  PRO H 257      37.299  31.268   9.136  1.00 20.14      H    C
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ATOM	3128	CG	PRO	H	257	38.684	31.608	8.721	1.00	20.11	H	C
ATOM	3129	CD	PRO	H	257	39.167	30.315	8.104	1.00	18.62	H	C
ATOM	3130	OT	PRO	H	257	36.786	31.886	6.001	1.00	26.65	H	O
ATOM	3131	N	THR	T	6	48.678	29.980	30.872	1.00	39.18	T	N
ATOM	3132	CA	THR	T	6	47.791	29.559	31.995	1.00	38.59	T	C
ATOM	3133	C	THR	T	6	47.976	28.083	32.299	1.00	36.71	T	C
ATOM	3134	O	THR	T	6	48.275	27.290	31.410	1.00	37.09	T	O
ATOM	3135	CB	THR	T	6	46.308	29.771	31.656	1.00	40.14	T	C
ATOM	3136	OG1	THR	T	6	45.930	28.877	30.600	1.00	41.93	T	O
ATOM	3137	CG2	THR	T	6	46.064	31.202	31.212	1.00	42.09	T	C
ATOM	3138	N	VAL	T	7	47.790	27.721	33.562	1.00	35.02	T	N
ATOM	3139	CA	VAL	T	7	47.919	26.335	33.987	1.00	33.21	T	C
ATOM	3140	C	VAL	T	7	46.611	25.871	34.613	1.00	31.57	T	C
ATOM	3141	O	VAL	T	7	45.876	26.663	35.211	1.00	31.61	T	O
ATOM	3142	CB	VAL	T	7	49.054	26.155	35.019	1.00	32.59	T	C
ATOM	3143	CG1	VAL	T	7	50.380	26.620	34.422	1.00	31.03	T	C
ATOM	3144	CG2	VAL	T	7	48.731	26.920	36.288	1.00	31.27	T	C
ATOM	3145	N	ALA	T	8	46.320	24.587	34.468	1.00	29.98	T	N
ATOM	3146	CA	ALA	T	8	45.101	24.023	35.023	1.00	29.21	T	C
ATOM	3147	C	ALA	T	8	45.239	23.892	36.531	1.00	28.58	T	C
ATOM	3148	O	ALA	T	8	46.342	23.743	37.055	1.00	28.70	T	O
ATOM	3149	CB	ALA	T	8	44.828	22.660	34.402	1.00	28.98	T	C
ATOM	3150	N	ALA	T	9	44.115	23.964	37.230	1.00	25.62	T	N
ATOM	3151	CA	ALA	T	9	44.121	23.828	38.673	1.00	25.80	T	C
ATOM	3152	C	ALA	T	9	44.490	22.387	39.016	1.00	26.18	T	C
ATOM	3153	O	ALA	T	9	44.425	21.501	38.161	1.00	25.07	T	O
ATOM	3154	CB	ALA	T	9	42.744	24.162	39.233	1.00	22.93	T	C
ATOM	3155	N	TYR	T	10	44.886	22.157	40.263	1.00	24.93	T	N
ATOM	3156	CA	TYR	T	10	45.240	20.815	40.701	1.00	25.50	T	C
ATOM	3157	C	TYR	T	10	44.978	20.661	42.186	1.00	25.20	T	C
ATOM	3158	O	TYR	T	10	44.754	21.641	42.896	1.00	23.18	T	O
ATOM	3159	CB	TYR	T	10	46.706	20.493	40.367	1.00	27.61	T	C
ATOM	3160	CG	TYR	T	10	47.724	21.429	40.975	1.00	27.41	T	C
ATOM	3161	CD1	TYR	T	10	48.245	21.199	42.248	1.00	28.54	T	C
ATOM	3162	CD2	TYR	T	10	48.160	22.554	40.277	1.00	28.91	T	C
ATOM	3163	CE1	TYR	T	10	49.183	22.072	42.810	1.00	28.45	T	C
ATOM	3164	CE2	TYR	T	10	49.090	23.429	40.827	1.00	29.62	T	C
ATOM	3165	CZ	TYR	T	10	49.595	23.184	42.088	1.00	29.24	T	C
ATOM	3166	OH	TYR	T	10	50.506	24.061	42.626	1.00	33.96	T	O
ATOM	3167	N	ASN	T	11	44.992	19.418	42.647	1.00	25.50	T	N
ATOM	3168	CA	ASN	T	11	44.729	19.119	44.045	1.00	25.22	T	C
ATOM	3169	C	ASN	T	11	43.354	19.624	44.466	1.00	23.78	T	C
ATOM	3170	O	ASN	T	11	43.197	20.179	45.553	1.00	20.92	T	O
ATOM	3171	CB	ASN	T	11	45.812	19.735	44.944	1.00	29.09	T	C
ATOM	3172	CG	ASN	T	11	47.105	18.924	44.954	1.00	31.48	T	C
ATOM	3173	OD1	ASN	T	11	48.090	19.321	45.578	1.00	34.70	T	O
ATOM	3174	ND2	ASN	T	11	47.105	17.784	44.270	1.00	32.60	T	N
ATOM	3175	N	LEU	T	12	42.356	19.441	43.602	1.00	23.43	T	N
ATOM	3176	CA	LEU	T	12	41.003	19.868	43.939	1.00	22.96	T	C
ATOM	3177	C	LEU	T	12	40.594	19.011	45.126	1.00	22.88	T	C
ATOM	3178	O	LEU	T	12	40.726	17.792	45.084	1.00	24.43	T	O
ATOM	3179	CB	LEU	T	12	40.043	19.652	42.763	1.00	21.46	T	C
ATOM	3180	CG	LEU	T	12	40.003	20.731	41.671	1.00	20.61	T	C
ATOM	3181	CD1	LEU	T	12	41.321	20.784	40.921	1.00	19.28	T	C
ATOM	3182	CD2	LEU	T	12	38.859	20.437	40.712	1.00	17.88	T	C
ATOM	3183	N	THR	T	13	40.097	19.651	46.178	1.00	22.51	T	N

ATOM	3184	CA	THR	T	13	39.719	18.946	47.394	1.00	22.60	T	C
ATOM	3185	C	THR	T	13	38.387	19.434	47.936	1.00	21.35	T	C
ATOM	3186	O	THR	T	13	38.106	20.622	47.904	1.00	22.14	T	O
ATOM	3187	CB	THR	T	13	40.786	19.172	48.494	1.00	24.31	T	C
ATOM	3188	OG1	THR	T	13	42.087	18.887	47.965	1.00	28.20	T	O
ATOM	3189	CG2	THR	T	13	40.524	18.276	49.695	1.00	25.13	T	C
ATOM	3190	N	TRP	T	14	37.570	18.517	48.442	1.00	20.93	T	N
ATOM	3191	CA	TRP	T	14	36.290	18.896	49.022	1.00	21.26	T	C
ATOM	3192	C	TRP	T	14	36.445	19.101	50.527	1.00	21.82	T	C
ATOM	3193	O	TRP	T	14	37.003	18.250	51.221	1.00	22.88	T	O
ATOM	3194	CB	TRP	T	14	35.233	17.816	48.775	1.00	21.62	T	C
ATOM	3195	CG	TRP	T	14	34.895	17.603	47.331	1.00	20.57	T	C
ATOM	3196	CD1	TRP	T	14	35.525	16.769	46.450	1.00	19.07	T	C
ATOM	3197	CD2	TRP	T	14	33.843	18.238	46.602	1.00	18.11	T	C
ATOM	3198	NE1	TRP	T	14	34.925	16.845	45.215	1.00	19.68	T	N
ATOM	3199	CE2	TRP	T	14	33.889	17.741	45.281	1.00	20.45	T	C
ATOM	3200	CE3	TRP	T	14	32.863	19.180	46.936	1.00	20.85	T	C
ATOM	3201	CZ2	TRP	T	14	32.989	18.155	44.292	1.00	20.30	T	C
ATOM	3202	CZ3	TRP	T	14	31.964	19.592	45.953	1.00	20.57	T	C
ATOM	3203	CH2	TRP	T	14	32.037	19.077	44.646	1.00	20.36	T	C
ATOM	3204	N	LYS	T	15	35.968	20.240	51.016	1.00	21.08	T	N
ATOM	3205	CA	LYS	T	15	36.005	20.568	52.439	1.00	20.11	T	C
ATOM	3206	C	LYS	T	15	34.534	20.651	52.818	1.00	19.45	T	C
ATOM	3207	O	LYS	T	15	33.862	21.632	52.510	1.00	20.83	T	O
ATOM	3208	CB	LYS	T	15	36.700	21.918	52.663	1.00	21.44	T	C
ATOM	3209	CG	LYS	T	15	38.162	21.933	52.228	1.00	23.27	T	C
ATOM	3210	CD	LYS	T	15	38.990	20.995	53.097	1.00	28.61	T	C
ATOM	3211	CE	LYS	T	15	40.296	20.589	52.427	1.00	31.74	T	C
ATOM	3212	NZ	LYS	T	15	41.190	21.741	52.152	1.00	36.85	T	N
ATOM	3213	N	SER	T	16	34.035	19.613	53.478	1.00	17.55	T	N
ATOM	3214	CA	SER	T	16	32.628	19.556	53.832	1.00	17.18	T	C
ATOM	3215	C	SER	T	16	32.363	19.073	55.255	1.00	18.04	T	C
ATOM	3216	O	SER	T	16	32.859	18.021	55.671	1.00	16.19	T	O
ATOM	3217	CB	SER	T	16	31.906	18.639	52.831	1.00	17.42	T	C
ATOM	3218	OG	SER	T	16	30.500	18.633	53.032	1.00	16.16	T	O
ATOM	3219	N	THR	T	17	31.572	19.851	55.988	1.00	17.33	T	N
ATOM	3220	CA	THR	T	17	31.199	19.523	57.360	1.00	17.85	T	C
ATOM	3221	C	THR	T	17	29.735	19.890	57.527	1.00	17.66	T	C
ATOM	3222	O	THR	T	17	29.345	21.033	57.293	1.00	17.63	T	O
ATOM	3223	CB	THR	T	17	32.031	20.322	58.385	1.00	16.36	T	C
ATOM	3224	OG1	THR	T	17	33.414	19.996	58.231	1.00	18.91	T	O
ATOM	3225	CG2	THR	T	17	31.596	19.990	59.799	1.00	17.35	T	C
ATOM	3226	N	ASN	T	18	28.922	18.922	57.935	1.00	18.02	T	N
ATOM	3227	CA	ASN	T	18	27.493	19.160	58.103	1.00	19.26	T	C
ATOM	3228	C	ASN	T	18	26.901	19.764	56.837	1.00	18.10	T	C
ATOM	3229	O	ASN	T	18	26.039	20.643	56.886	1.00	18.37	T	O
ATOM	3230	CB	ASN	T	18	27.238	20.073	59.301	1.00	20.54	T	C
ATOM	3231	CG	ASN	T	18	27.792	19.494	60.579	1.00	23.12	T	C
ATOM	3232	OD1	ASN	T	18	27.706	18.288	60.804	1.00	22.01	T	O
ATOM	3233	ND2	ASN	T	18	28.368	20.346	61.423	1.00	26.13	T	N
ATOM	3234	N	PHE	T	19	27.394	19.269	55.706	1.00	18.27	T	N
ATOM	3235	CA	PHE	T	19	26.959	19.672	54.383	1.00	19.15	T	C
ATOM	3236	C	PHE	T	19	27.453	21.022	53.869	1.00	20.26	T	C
ATOM	3237	O	PHE	T	19	27.200	21.369	52.715	1.00	20.39	T	O
ATOM	3238	CB	PHE	T	19	25.441	19.539	54.305	1.00	20.26	T	C
ATOM	3239	CG	PHE	T	19	24.965	18.124	54.530	1.00	21.59	T	C

ATOM	3240	CD1	PHE	T	19	25.184	17.144	53.565	1.00	21.66	T	C
ATOM	3241	CD2	PHE	T	19	24.371	17.755	55.731	1.00	22.37	T	C
ATOM	3242	CE1	PHE	T	19	24.823	15.819	53.790	1.00	21.75	T	C
ATOM	3243	CE2	PHE	T	19	24.003	16.425	55.970	1.00	24.36	T	C
ATOM	3244	CZ	PHE	T	19	24.232	15.456	54.995	1.00	22.96	T	C
ATOM	3245	N	LYS	T	20	28.162	21.779	54.706	1.00	19.77	T	N
ATOM	3246	CA	LYS	T	20	28.737	23.044	54.252	1.00	18.78	T	C
ATOM	3247	C	LYS	T	20	29.855	22.526	53.362	1.00	18.12	T	C
ATOM	3248	O	LYS	T	20	30.848	21.993	53.853	1.00	19.69	T	O
ATOM	3249	CB	LYS	T	20	29.326	23.831	55.414	1.00	20.11	T	C
ATOM	3250	CG	LYS	T	20	28.777	25.232	55.535	1.00	22.19	T	C
ATOM	3251	CD	LYS	T	20	29.115	26.090	54.338	1.00	21.31	T	C
ATOM	3252	CE	LYS	T	20	28.434	27.437	54.474	1.00	21.39	T	C
ATOM	3253	NZ	LYS	T	20	28.973	28.453	53.548	1.00	23.07	T	N
ATOM	3254	N	THR	T	21	29.692	22.684	52.056	1.00	16.64	T	N
ATOM	3255	CA	THR	T	21	30.643	22.143	51.100	1.00	16.45	T	C
ATOM	3256	C	THR	T	21	31.364	23.167	50.243	1.00	18.19	T	C
ATOM	3257	O	THR	T	21	30.749	23.879	49.453	1.00	17.44	T	O
ATOM	3258	CB	THR	T	21	29.911	21.151	50.192	1.00	15.26	T	C
ATOM	3259	OG1	THR	T	21	29.179	20.236	51.016	1.00	16.35	T	O
ATOM	3260	CG2	THR	T	21	30.885	20.380	49.320	1.00	16.11	T	C
ATOM	3261	N	ILE	T	22	32.682	23.215	50.394	1.00	19.00	T	N
ATOM	3262	CA	ILE	T	22	33.511	24.146	49.648	1.00	19.12	T	C
ATOM	3263	C	ILE	T	22	34.603	23.396	48.896	1.00	18.47	T	C
ATOM	3264	O	ILE	T	22	35.326	22.588	49.477	1.00	18.08	T	O
ATOM	3265	CB	ILE	T	22	34.180	25.169	50.597	1.00	20.41	T	C
ATOM	3266	CG1	ILE	T	22	33.108	25.959	51.353	1.00	21.22	T	C
ATOM	3267	CG2	ILE	T	22	35.075	26.121	49.804	1.00	19.96	T	C
ATOM	3268	CD1	ILE	T	22	33.673	26.948	52.352	1.00	21.24	T	C
ATOM	3269	N	LEU	T	23	34.711	23.658	47.599	1.00	17.48	T	N
ATOM	3270	CA	LEU	T	23	35.738	23.029	46.783	1.00	18.70	T	C
ATOM	3271	C	LEU	T	23	36.967	23.925	46.847	1.00	17.63	T	C
ATOM	3272	O	LEU	T	23	36.859	25.141	46.691	1.00	18.29	T	O
ATOM	3273	CB	LEU	T	23	35.275	22.905	45.329	1.00	19.42	T	C
ATOM	3274	CG	LEU	T	23	36.258	22.183	44.399	1.00	21.43	T	C
ATOM	3275	CD1	LEU	T	23	36.325	20.714	44.790	1.00	19.69	T	C
ATOM	3276	CD2	LEU	T	23	35.820	22.334	42.944	1.00	17.72	T	C
ATOM	3277	N	GLU	T	24	38.129	23.334	47.093	1.00	16.78	T	N
ATOM	3278	CA	GLU	T	24	39.367	24.102	47.165	1.00	18.87	T	C
ATOM	3279	C	GLU	T	24	40.354	23.566	46.146	1.00	20.20	T	C
ATOM	3280	O	GLU	T	24	40.262	22.411	45.735	1.00	20.83	T	O
ATOM	3281	CB	GLU	T	24	39.968	24.025	48.575	1.00	18.72	T	C
ATOM	3282	CG	GLU	T	24	39.349	25.019	49.553	1.00	21.38	T	C
ATOM	3283	CD	GLU	T	24	39.777	24.789	50.988	1.00	23.65	T	C
ATOM	3284	OE1	GLU	T	24	40.878	24.291	51.202	1.00	25.81	T	O
ATOM	3285	OE2	GLU	T	24	39.008	25.125	51.887	1.00	26.26	T	O
ATOM	3286	N	TRP	T	25	41.300	24.401	45.735	1.00	19.89	T	N
ATOM	3287	CA	TRP	T	25	42.280	23.965	44.759	1.00	20.95	T	C
ATOM	3288	C	TRP	T	25	43.524	24.843	44.721	1.00	22.24	T	C
ATOM	3289	O	TRP	T	25	43.635	25.829	45.451	1.00	23.01	T	O
ATOM	3290	CB	TRP	T	25	41.629	23.912	43.366	1.00	18.38	T	C
ATOM	3291	CG	TRP	T	25	41.213	25.252	42.815	1.00	16.29	T	C
ATOM	3292	CD1	TRP	T	25	41.994	26.133	42.115	1.00	16.76	T	C
ATOM	3293	CD2	TRP	T	25	39.917	25.856	42.911	1.00	14.79	T	C
ATOM	3294	NE1	TRP	T	25	41.260	27.246	41.765	1.00	13.11	T	N
ATOM	3295	CE2	TRP	T	25	39.984	27.102	42.242	1.00	14.48	T	C

ATOM	3296	CE3	TRP	T	25	38.704	25.466	43.498	1.00	15.24	T	C
ATOM	3297	CZ2	TRP	T	25	38.882	27.960	42.141	1.00	14.18	T	C
ATOM	3298	CZ3	TRP	T	25	37.606	26.320	43.399	1.00	14.21	T	C
ATOM	3299	CH2	TRP	T	25	37.705	27.554	42.725	1.00	15.19	T	C
ATOM	3300	N	GLU	T	26	44.455	24.449	43.862	1.00	24.44	T	N
ATOM	3301	CA	GLU	T	26	45.713	25.148	43.644	1.00	27.06	T	C
ATOM	3302	C	GLU	T	26	45.713	25.499	42.159	1.00	28.34	T	C
ATOM	3303	O	GLU	T	26	44.953	24.918	41.384	1.00	26.89	T	O
ATOM	3304	CB	GLU	T	26	46.889	24.214	43.939	1.00	28.64	T	C
ATOM	3305	CG	GLU	T	26	46.993	23.741	45.376	1.00	34.94	T	C
ATOM	3306	CD	GLU	T	26	47.761	24.705	46.253	1.00	39.39	T	C
ATOM	3307	OE1	GLU	T	26	47.870	24.444	47.440	1.00	42.73	T	O
ATOM	3308	OE2	GLU	T	26	48.255	25.713	45.739	1.00	42.24	T	O
ATOM	3309	N	PRO	T	27	46.567	26.445	41.737	1.00	30.61	T	N
ATOM	3310	CA	PRO	T	27	47.516	27.202	42.550	1.00	33.08	T	C
ATOM	3311	C	PRO	T	27	47.039	28.646	42.694	1.00	36.39	T	C
ATOM	3312	O	PRO	T	27	45.969	29.008	42.204	1.00	37.38	T	O
ATOM	3313	CB	PRO	T	27	48.781	27.116	41.722	1.00	31.05	T	C
ATOM	3314	CG	PRO	T	27	48.232	27.369	40.350	1.00	29.94	T	C
ATOM	3315	CD	PRO	T	27	46.943	26.535	40.312	1.00	29.62	T	C
ATOM	3316	N	LYS	T	28	47.844	29.469	43.354	1.00	40.49	T	N
ATOM	3317	CA	LYS	T	28	47.509	30.874	43.534	1.00	44.79	T	C
ATOM	3318	C	LYS	T	28	47.525	31.555	42.169	1.00	46.88	T	C
ATOM	3319	O	LYS	T	28	48.585	31.737	41.566	1.00	47.96	T	O
ATOM	3320	CB	LYS	T	28	48.518	31.537	44.472	1.00	45.11	T	C
ATOM	3321	CG	LYS	T	28	48.533	30.923	45.859	1.00	46.65	T	C
ATOM	3322	CD	LYS	T	28	47.146	30.969	46.483	1.00	47.76	T	C
ATOM	3323	CE	LYS	T	28	47.120	30.295	47.843	1.00	49.21	T	C
ATOM	3324	NZ	LYS	T	28	45.769	30.375	48.468	1.00	50.84	T	N
ATOM	3325	N	PRO	T	29	46.342	31.942	41.667	1.00	47.94	T	N
ATOM	3326	CA	PRO	T	29	46.170	32.602	40.371	1.00	48.83	T	C
ATOM	3327	C	PRO	T	29	47.026	33.841	40.130	1.00	49.78	T	C
ATOM	3328	O	PRO	T	29	46.997	34.802	40.899	1.00	49.58	T	O
ATOM	3329	CB	PRO	T	29	44.677	32.914	40.339	1.00	48.24	T	C
ATOM	3330	CG	PRO	T	29	44.346	33.102	41.778	1.00	47.36	T	C
ATOM	3331	CD	PRO	T	29	45.074	31.952	42.417	1.00	48.57	T	C
ATOM	3332	N	VAL	T	30	47.790	33.795	39.044	1.00	50.46	T	N
ATOM	3333	CA	VAL	T	30	48.656	34.894	38.640	1.00	51.62	T	C
ATOM	3334	C	VAL	T	30	48.245	35.208	37.210	1.00	51.40	T	C
ATOM	3335	O	VAL	T	30	48.602	34.479	36.283	1.00	51.31	T	O
ATOM	3336	CB	VAL	T	30	50.138	34.482	38.664	1.00	51.98	T	C
ATOM	3337	CG1	VAL	T	30	51.002	35.657	38.258	1.00	52.42	T	C
ATOM	3338	CG2	VAL	T	30	50.523	33.993	40.055	1.00	51.87	T	C
ATOM	3339	N	ASN	T	31	47.491	36.291	37.033	1.00	50.80	T	N
ATOM	3340	CA	ASN	T	31	46.994	36.652	35.709	1.00	49.64	T	C
ATOM	3341	C	ASN	T	31	46.213	35.437	35.222	1.00	46.82	T	C
ATOM	3342	O	ASN	T	31	46.349	35.007	34.077	1.00	46.96	T	O
ATOM	3343	CB	ASN	T	31	48.155	36.952	34.760	1.00	52.08	T	C
ATOM	3344	CG	ASN	T	31	48.857	38.249	35.095	1.00	54.19	T	C
ATOM	3345	OD1	ASN	T	31	48.257	39.322	35.032	1.00	56.94	T	O
ATOM	3346	ND2	ASN	T	31	50.131	38.160	35.457	1.00	54.94	T	N
ATOM	3347	N	GLN	T	32	45.392	34.897	36.118	1.00	44.02	T	N
ATOM	3348	CA	GLN	T	32	44.597	33.711	35.845	1.00	39.84	T	C
ATOM	3349	C	GLN	T	32	43.356	33.696	36.732	1.00	36.22	T	C
ATOM	3350	O	GLN	T	32	43.450	33.789	37.956	1.00	36.42	T	O
ATOM	3351	CB	GLN	T	32	45.457	32.474	36.107	1.00	40.02	T	C

ATOM	3352	CG	GLN	T	32	44.756	31.141	35.996	1.00	38.97	T	C
ATOM	3353	CD	GLN	T	32	45.743	29.991	36.046	1.00	37.53	T	C
ATOM	3354	OE1	GLN	T	32	46.616	29.880	35.189	1.00	36.12	T	O
ATOM	3355	NE2	GLN	T	32	45.614	29.136	37.053	1.00	35.32	T	N
ATOM	3356	N	VAL	T	33	42.192	33.578	36.104	1.00	31.20	T	N
ATOM	3357	CA	VAL	T	33	40.930	33.555	36.824	1.00	26.24	T	C
ATOM	3358	C	VAL	T	33	40.280	32.178	36.683	1.00	24.67	T	C
ATOM	3359	O	VAL	T	33	40.698	31.375	35.851	1.00	23.37	T	O
ATOM	3360	CB	VAL	T	33	39.986	34.658	36.296	1.00	25.12	T	C
ATOM	3361	CG1	VAL	T	33	40.676	36.014	36.410	1.00	23.86	T	C
ATOM	3362	CG2	VAL	T	33	39.603	34.385	34.854	1.00	26.27	T	C
ATOM	3363	N	TYR	T	34	39.260	31.911	37.493	1.00	21.25	T	N
ATOM	3364	CA	TYR	T	34	38.589	30.615	37.473	1.00	19.35	T	C
ATOM	3365	C	TYR	T	34	37.070	30.677	37.428	1.00	18.92	T	C
ATOM	3366	O	TYR	T	34	36.454	31.670	37.801	1.00	18.57	T	O
ATOM	3367	CB	TYR	T	34	38.947	29.816	38.728	1.00	18.40	T	C
ATOM	3368	CG	TYR	T	34	40.416	29.582	38.957	1.00	20.44	T	C
ATOM	3369	CD1	TYR	T	34	41.125	28.667	38.182	1.00	18.46	T	C
ATOM	3370	CD2	TYR	T	34	41.096	30.259	39.971	1.00	19.10	T	C
ATOM	3371	CE1	TYR	T	34	42.475	28.424	38.412	1.00	19.96	T	C
ATOM	3372	CE2	TYR	T	34	42.447	30.021	40.207	1.00	20.05	T	C
ATOM	3373	CZ	TYR	T	34	43.126	29.102	39.426	1.00	20.10	T	C
ATOM	3374	OH	TYR	T	34	44.454	28.848	39.669	1.00	24.65	T	O
ATOM	3375	N	THR	T	35	36.478	29.581	36.974	1.00	16.56	T	N
ATOM	3376	CA	THR	T	35	35.034	29.429	36.956	1.00	16.37	T	C
ATOM	3377	C	THR	T	35	34.831	27.950	37.233	1.00	15.30	T	C
ATOM	3378	O	THR	T	35	35.490	27.103	36.634	1.00	18.13	T	O
ATOM	3379	CB	THR	T	35	34.390	29.799	35.608	1.00	15.23	T	C
ATOM	3380	OG1	THR	T	35	34.409	31.222	35.438	1.00	15.18	T	O
ATOM	3381	CG2	THR	T	35	32.941	29.336	35.581	1.00	16.79	T	C
ATOM	3382	N	VAL	T	36	33.940	27.647	38.163	1.00	15.22	T	N
ATOM	3383	CA	VAL	T	36	33.669	26.271	38.543	1.00	14.65	T	C
ATOM	3384	C	VAL	T	36	32.340	25.787	37.974	1.00	14.97	T	C
ATOM	3385	O	VAL	T	36	31.405	26.568	37.816	1.00	15.99	T	O
ATOM	3386	CB	VAL	T	36	33.638	26.153	40.086	1.00	12.56	T	C
ATOM	3387	CG1	VAL	T	36	33.230	24.751	40.517	1.00	14.14	T	C
ATOM	3388	CG2	VAL	T	36	35.019	26.496	40.652	1.00	13.80	T	C
ATOM	3389	N	GLN	T	37	32.278	24.507	37.624	1.00	14.43	T	N
ATOM	3390	CA	GLN	T	37	31.045	23.903	37.136	1.00	14.45	T	C
ATOM	3391	C	GLN	T	37	30.796	22.668	37.990	1.00	14.47	T	C
ATOM	3392	O	GLN	T	37	31.733	21.976	38.381	1.00	14.12	T	O
ATOM	3393	CB	GLN	T	37	31.152	23.468	35.671	1.00	14.86	T	C
ATOM	3394	CG	GLN	T	37	31.085	24.583	34.637	1.00	14.48	T	C
ATOM	3395	CD	GLN	T	37	30.857	24.037	33.234	1.00	13.74	T	C
ATOM	3396	OE1	GLN	T	37	31.300	22.940	32.912	1.00	13.95	T	O
ATOM	3397	NE2	GLN	T	37	30.175	24.807	32.393	1.00	10.80	T	N
ATOM	3398	N	ILE	T	38	29.533	22.399	38.287	1.00	14.90	T	N
ATOM	3399	CA	ILE	T	38	29.176	21.231	39.070	1.00	14.60	T	C
ATOM	3400	C	ILE	T	38	27.965	20.576	38.417	1.00	16.38	T	C
ATOM	3401	O	ILE	T	38	27.150	21.252	37.788	1.00	17.10	T	O
ATOM	3402	CB	ILE	T	38	28.829	21.617	40.521	1.00	15.19	T	C
ATOM	3403	CG1	ILE	T	38	28.607	20.351	41.358	1.00	14.88	T	C
ATOM	3404	CG2	ILE	T	38	27.601	22.530	40.539	1.00	10.78	T	C
ATOM	3405	CD1	ILE	T	38	28.402	20.620	42.845	1.00	14.77	T	C
ATOM	3406	N	SER	T	39	27.857	19.260	38.557	1.00	16.00	T	N
ATOM	3407	CA	SER	T	39	26.737	18.529	37.989	1.00	15.27	T	C

ATOM	3408	C	SER	T	39	26.642	17.157	38.622	1.00	15.45	T	C
ATOM	3409	O	SER	T	39	27.511	16.748	39.382	1.00	16.91	T	O
ATOM	3410	CB	SER	T	39	26.948	18.327	36.491	1.00	12.90	T	C
ATOM	3411	OG	SER	T	39	27.999	17.389	36.285	1.00	12.71	T	O
ATOM	3412	N	THR	T	40	25.569	16.453	38.295	1.00	17.91	T	N
ATOM	3413	CA	THR	T	40	25.381	15.088	38.745	1.00	18.74	T	C
ATOM	3414	C	THR	T	40	25.637	14.283	37.480	1.00	21.10	T	C
ATOM	3415	O	THR	T	40	25.606	14.839	36.378	1.00	20.86	T	O
ATOM	3416	CB	THR	T	40	23.947	14.834	39.245	1.00	19.11	T	C
ATOM	3417	OG1	THR	T	40	23.002	15.399	38.325	1.00	17.75	T	O
ATOM	3418	CG2	THR	T	40	23.755	15.448	40.620	1.00	17.44	T	C
ATOM	3419	N	LYS	T	41	25.896	12.989	37.639	1.00	24.75	T	N
ATOM	3420	CA	LYS	T	41	26.183	12.079	36.527	1.00	26.61	T	C
ATOM	3421	C	LYS	T	41	25.427	12.345	35.224	1.00	26.89	T	C
ATOM	3422	O	LYS	T	41	26.032	12.422	34.154	1.00	27.99	T	O
ATOM	3423	CB	LYS	T	41	25.922	10.637	36.970	1.00	31.82	T	C
ATOM	3424	CG	LYS	T	41	26.089	9.598	35.873	1.00	37.07	T	C
ATOM	3425	CD	LYS	T	41	25.717	8.204	36.371	1.00	39.57	T	C
ATOM	3426	CE	LYS	T	41	25.812	7.175	35.253	1.00	40.27	T	C
ATOM	3427	NZ	LYS	T	41	25.454	5.808	35.729	1.00	43.52	T	N
ATOM	3428	N	SER	T	42	24.108	12.473	35.303	1.00	24.42	T	N
ATOM	3429	CA	SER	T	42	23.324	12.711	34.105	1.00	24.61	T	C
ATOM	3430	C	SER	T	42	22.618	14.066	34.081	1.00	22.94	T	C
ATOM	3431	O	SER	T	42	21.641	14.244	33.360	1.00	25.38	T	O
ATOM	3432	CB	SER	T	42	22.299	11.588	33.926	1.00	26.04	T	C
ATOM	3433	OG	SER	T	42	21.442	11.505	35.048	1.00	31.07	T	O
ATOM	3434	N	GLY	T	43	23.114	15.017	34.866	1.00	19.49	T	N
ATOM	3435	CA	GLY	T	43	22.513	16.338	34.898	1.00	18.07	T	C
ATOM	3436	C	GLY	T	43	23.352	17.340	34.125	1.00	15.78	T	C
ATOM	3437	O	GLY	T	43	24.494	17.058	33.774	1.00	15.61	T	O
ATOM	3438	N	ASP	T	44	22.787	18.508	33.852	1.00	15.33	T	N
ATOM	3439	CA	ASP	T	44	23.500	19.543	33.119	1.00	15.18	T	C
ATOM	3440	C	ASP	T	44	24.586	20.168	33.991	1.00	15.75	T	C
ATOM	3441	O	ASP	T	44	24.536	20.085	35.220	1.00	14.67	T	O
ATOM	3442	CB	ASP	T	44	22.532	20.645	32.664	1.00	14.49	T	C
ATOM	3443	CG	ASP	T	44	21.512	20.163	31.635	1.00	15.31	T	C
ATOM	3444	OD1	ASP	T	44	21.724	19.121	31.012	1.00	11.39	T	O
ATOM	3445	OD2	ASP	T	44	20.500	20.857	31.448	1.00	16.14	T	O
ATOM	3446	N	TRP	T	45	25.570	20.794	33.356	1.00	15.26	T	N
ATOM	3447	CA	TRP	T	45	26.632	21.449	34.104	1.00	16.12	T	C
ATOM	3448	C	TRP	T	45	26.155	22.832	34.532	1.00	16.65	T	C
ATOM	3449	O	TRP	T	45	25.592	23.575	33.738	1.00	17.64	T	O
ATOM	3450	CB	TRP	T	45	27.895	21.576	33.259	1.00	14.65	T	C
ATOM	3451	CG	TRP	T	45	28.542	20.254	32.967	1.00	16.11	T	C
ATOM	3452	CD1	TRP	T	45	28.359	19.476	31.859	1.00	14.82	T	C
ATOM	3453	CD2	TRP	T	45	29.469	19.550	33.804	1.00	15.28	T	C
ATOM	3454	NE1	TRP	T	45	29.119	18.332	31.951	1.00	14.03	T	N
ATOM	3455	CE2	TRP	T	45	29.812	18.352	33.135	1.00	15.34	T	C
ATOM	3456	CE3	TRP	T	45	30.044	19.814	35.056	1.00	17.68	T	C
ATOM	3457	CZ2	TRP	T	45	30.708	17.420	33.672	1.00	14.08	T	C
ATOM	3458	CZ3	TRP	T	45	30.938	18.884	35.595	1.00	15.15	T	C
ATOM	3459	CH2	TRP	T	45	31.260	17.703	34.899	1.00	15.49	T	C
ATOM	3460	N	LYS	T	46	26.374	23.165	35.795	1.00	16.58	T	N
ATOM	3461	CA	LYS	T	46	25.960	24.455	36.323	1.00	17.49	T	C
ATOM	3462	C	LYS	T	46	27.218	25.240	36.702	1.00	16.41	T	C
ATOM	3463	O	LYS	T	46	28.109	24.704	37.358	1.00	17.90	T	O

ATOM	3464	CB	LYS	T	46	25.070	24.223	37.545	1.00	18.63	T	C
ATOM	3465	CG	LYS	T	46	24.011	25.285	37.794	1.00	25.36	T	C
ATOM	3466	CD	LYS	T	46	24.421	26.245	38.886	1.00	27.44	T	C
ATOM	3467	CE	LYS	T	46	23.245	27.096	39.336	1.00	30.02	T	C
ATOM	3468	NZ	LYS	T	46	22.215	26.308	40.063	1.00	30.73	T	N
ATOM	3469	N	SER	T	47	27.299	26.499	36.276	1.00	16.11	T	N
ATOM	3470	CA	SER	T	47	28.460	27.334	36.582	1.00	14.72	T	C
ATOM	3471	C	SER	T	47	28.330	28.031	37.928	1.00	13.96	T	C
ATOM	3472	O	SER	T	47	27.244	28.454	38.319	1.00	13.03	T	O
ATOM	3473	CB	SER	T	47	28.678	28.386	35.488	1.00	11.64	T	C
ATOM	3474	OG	SER	T	47	29.306	27.819	34.350	1.00	15.92	T	O
ATOM	3475	N	LYS	T	48	29.456	28.163	38.619	1.00	13.74	T	N
ATOM	3476	CA	LYS	T	48	29.503	28.794	39.935	1.00	15.63	T	C
ATOM	3477	C	LYS	T	48	30.801	29.581	40.095	1.00	15.18	T	C
ATOM	3478	O	LYS	T	48	31.774	29.346	39.376	1.00	14.77	T	O
ATOM	3479	CB	LYS	T	48	29.447	27.724	41.033	1.00	13.97	T	C
ATOM	3480	CG	LYS	T	48	28.293	26.747	40.906	1.00	15.98	T	C
ATOM	3481	CD	LYS	T	48	27.363	26.832	42.093	1.00	19.94	T	C
ATOM	3482	CE	LYS	T	48	26.789	28.221	42.253	1.00	19.83	T	C
ATOM	3483	NZ	LYS	T	48	25.892	28.306	43.425	1.00	18.63	T	N
ATOM	3484	N	CYS	T	49	30.806	30.508	41.046	1.00	16.26	T	N
ATOM	3485	CA	CYS	T	49	31.993	31.308	41.339	1.00	17.07	T	C
ATOM	3486	C	CYS	T	49	32.635	31.844	40.058	1.00	17.80	T	C
ATOM	3487	O	CYS	T	49	33.815	31.627	39.784	1.00	17.68	T	O
ATOM	3488	CB	CYS	T	49	32.975	30.448	42.144	1.00	15.94	T	C
ATOM	3489	SG	CYS	T	49	32.249	29.824	43.705	1.00	18.32	T	S
ATOM	3490	N	PHE	T	50	31.826	32.568	39.293	1.00	19.09	T	N
ATOM	3491	CA	PHE	T	50	32.208	33.145	38.006	1.00	19.69	T	C
ATOM	3492	C	PHE	T	50	33.438	34.046	38.020	1.00	18.93	T	C
ATOM	3493	O	PHE	T	50	33.462	35.073	38.687	1.00	19.65	T	O
ATOM	3494	CB	PHE	T	50	31.018	33.925	37.437	1.00	21.03	T	C
ATOM	3495	CG	PHE	T	50	29.705	33.212	37.598	1.00	22.82	T	C
ATOM	3496	CD1	PHE	T	50	29.410	32.090	36.834	1.00	23.21	T	C
ATOM	3497	CD2	PHE	T	50	28.791	33.626	38.562	1.00	24.00	T	C
ATOM	3498	CE1	PHE	T	50	28.225	31.388	37.031	1.00	22.86	T	C
ATOM	3499	CE2	PHE	T	50	27.604	32.929	38.768	1.00	24.77	T	C
ATOM	3500	CZ	PHE	T	50	27.324	31.808	38.000	1.00	24.10	T	C
ATOM	3501	N	TYR	T	51	34.454	33.646	37.264	1.00	19.61	T	N
ATOM	3502	CA	TYR	T	51	35.694	34.404	37.135	1.00	19.80	T	C
ATOM	3503	C	TYR	T	51	36.262	34.886	38.459	1.00	20.72	T	C
ATOM	3504	O	TYR	T	51	36.662	36.043	38.590	1.00	20.88	T	O
ATOM	3505	CB	TYR	T	51	35.470	35.601	36.212	1.00	20.21	T	C
ATOM	3506	CG	TYR	T	51	34.778	35.245	34.915	1.00	21.19	T	C
ATOM	3507	CD1	TYR	T	51	35.358	34.354	34.011	1.00	20.94	T	C
ATOM	3508	CD2	TYR	T	51	33.536	35.795	34.596	1.00	22.01	T	C
ATOM	3509	CE1	TYR	T	51	34.717	34.021	32.820	1.00	23.56	T	C
ATOM	3510	CE2	TYR	T	51	32.888	35.471	33.409	1.00	23.16	T	C
ATOM	3511	CZ	TYR	T	51	33.481	34.586	32.527	1.00	25.31	T	C
ATOM	3512	OH	TYR	T	51	32.835	34.271	31.353	1.00	29.02	T	O
ATOM	3513	N	THR	T	52	36.300	33.989	39.436	1.00	20.20	T	N
ATOM	3514	CA	THR	T	52	36.828	34.301	40.754	1.00	19.96	T	C
ATOM	3515	C	THR	T	52	38.348	34.188	40.741	1.00	20.71	T	C
ATOM	3516	O	THR	T	52	38.916	33.409	39.970	1.00	19.97	T	O
ATOM	3517	CB	THR	T	52	36.283	33.317	41.816	1.00	19.38	T	C
ATOM	3518	OG1	THR	T	52	36.848	33.631	43.094	1.00	18.27	T	O
ATOM	3519	CG2	THR	T	52	36.651	31.878	41.452	1.00	20.27	T	C

ATOM	3520	N	THR	T	53	39.007	34.973	41.585	1.00	20.41	T	N
ATOM	3521	CA	THR	T	53	40.460	34.911	41.688	1.00	22.43	T	C
ATOM	3522	C	THR	T	53	40.862	34.112	42.934	1.00	23.31	T	C
ATOM	3523	O	THR	T	53	42.042	33.872	43.178	1.00	24.50	T	O
ATOM	3524	CB	THR	T	53	41.094	36.318	41.751	1.00	21.43	T	C
ATOM	3525	OG1	THR	T	53	40.475	37.077	42.793	1.00	23.60	T	O
ATOM	3526	CG2	THR	T	53	40.919	37.039	40.423	1.00	20.43	T	C
ATOM	3527	N	ASP	T	54	39.878	33.701	43.727	1.00	24.66	T	N
ATOM	3528	CA	ASP	T	54	40.170	32.907	44.910	1.00	24.86	T	C
ATOM	3529	C	ASP	T	54	40.341	31.467	44.447	1.00	24.57	T	C
ATOM	3530	O	ASP	T	54	39.991	31.124	43.311	1.00	23.26	T	O
ATOM	3531	CB	ASP	T	54	39.027	32.991	45.920	1.00	28.59	T	C
ATOM	3532	CG	ASP	T	54	38.695	34.418	46.307	1.00	31.77	T	C
ATOM	3533	OD1	ASP	T	54	39.607	35.179	46.642	1.00	35.02	T	O
ATOM	3534	OD2	ASP	T	54	37.529	34.759	46.279	1.00	36.17	T	O
ATOM	3535	N	THR	T	55	40.888	30.625	45.316	1.00	20.61	T	N
ATOM	3536	CA	THR	T	55	41.088	29.230	44.969	1.00	18.26	T	C
ATOM	3537	C	THR	T	55	40.114	28.339	45.741	1.00	18.54	T	C
ATOM	3538	O	THR	T	55	40.483	27.264	46.222	1.00	16.66	T	O
ATOM	3539	CB	THR	T	55	42.526	28.806	45.266	1.00	17.06	T	C
ATOM	3540	OG1	THR	T	55	42.852	29.159	46.612	1.00	17.45	T	O
ATOM	3541	CG2	THR	T	55	43.488	29.500	44.321	1.00	19.50	T	C
ATOM	3542	N	GLU	T	56	38.871	28.804	45.857	1.00	15.86	T	N
ATOM	3543	CA	GLU	T	56	37.822	28.072	46.553	1.00	17.50	T	C
ATOM	3544	C	GLU	T	56	36.462	28.477	45.999	1.00	16.59	T	C
ATOM	3545	O	GLU	T	56	36.294	29.576	45.475	1.00	15.56	T	O
ATOM	3546	CB	GLU	T	56	37.837	28.387	48.053	1.00	17.92	T	C
ATOM	3547	CG	GLU	T	56	37.396	29.809	48.374	1.00	20.51	T	C
ATOM	3548	CD	GLU	T	56	37.265	30.061	49.859	1.00	24.03	T	C
ATOM	3549	OE1	GLU	T	56	38.221	29.802	50.582	1.00	26.81	T	O
ATOM	3550	OE2	GLU	T	56	36.205	30.518	50.287	1.00	26.27	T	O
ATOM	3551	N	CYS	T	57	35.490	27.586	46.129	1.00	16.04	T	N
ATOM	3552	CA	CYS	T	57	34.147	27.870	45.665	1.00	16.17	T	C
ATOM	3553	C	CYS	T	57	33.140	27.164	46.552	1.00	15.98	T	C
ATOM	3554	O	CYS	T	57	33.225	25.954	46.754	1.00	14.72	T	O
ATOM	3555	CB	CYS	T	57	33.963	27.403	44.219	1.00	17.24	T	C
ATOM	3556	SG	CYS	T	57	32.314	27.793	43.557	1.00	17.97	T	S
ATOM	3557	N	ASP	T	58	32.187	27.918	47.084	1.00	14.99	T	N
ATOM	3558	CA	ASP	T	58	31.172	27.326	47.934	1.00	15.94	T	C
ATOM	3559	C	ASP	T	58	30.115	26.677	47.061	1.00	16.95	T	C
ATOM	3560	O	ASP	T	58	29.477	27.340	46.244	1.00	17.86	T	O
ATOM	3561	CB	ASP	T	58	30.526	28.385	48.829	1.00	16.18	T	C
ATOM	3562	CG	ASP	T	58	29.436	27.806	49.715	1.00	17.55	T	C
ATOM	3563	OD1	ASP	T	58	29.529	26.636	50.053	1.00	15.23	T	O
ATOM	3564	OD2	ASP	T	58	28.502	28.531	50.073	1.00	18.41	T	O
ATOM	3565	N	LEU	T	59	29.939	25.373	47.227	1.00	16.87	T	N
ATOM	3566	CA	LEU	T	59	28.951	24.643	46.449	1.00	16.97	T	C
ATOM	3567	C	LEU	T	59	27.832	24.092	47.331	1.00	17.59	T	C
ATOM	3568	O	LEU	T	59	27.077	23.218	46.916	1.00	19.55	T	O
ATOM	3569	CB	LEU	T	59	29.638	23.513	45.682	1.00	14.54	T	C
ATOM	3570	CG	LEU	T	59	30.694	24.010	44.686	1.00	16.18	T	C
ATOM	3571	CD1	LEU	T	59	31.435	22.828	44.072	1.00	13.02	T	C
ATOM	3572	CD2	LEU	T	59	30.019	24.850	43.606	1.00	14.07	T	C
ATOM	3573	N	THR	T	60	27.718	24.630	48.541	1.00	18.48	T	N
ATOM	3574	CA	THR	T	60	26.701	24.199	49.495	1.00	20.05	T	C
ATOM	3575	C	THR	T	60	25.274	24.228	48.952	1.00	20.61	T	C

ATOM	3576	O	THR	T	60	24.558	23.230	49.030	1.00	20.04	T	O
ATOM	3577	CB	THR	T	60	26.748	25.062	50.779	1.00	20.92	T	C
ATOM	3578	OG1	THR	T	60	28.024	24.909	51.415	1.00	21.02	T	O
ATOM	3579	CG2	THR	T	60	25.654	24.647	51.747	1.00	19.78	T	C
ATOM	3580	N	ASP	T	61	24.859	25.368	48.405	1.00	20.95	T	N
ATOM	3581	CA	ASP	T	61	23.500	25.507	47.884	1.00	22.33	T	C
ATOM	3582	C	ASP	T	61	23.142	24.529	46.778	1.00	21.88	T	C
ATOM	3583	O	ASP	T	61	21.967	24.220	46.574	1.00	23.89	T	O
ATOM	3584	CB	ASP	T	61	23.252	26.934	47.391	1.00	23.16	T	C
ATOM	3585	CG	ASP	T	61	23.321	27.947	48.507	1.00	26.60	T	C
ATOM	3586	OD1	ASP	T	61	23.175	27.550	49.659	1.00	28.12	T	O
ATOM	3587	OD2	ASP	T	61	23.511	29.127	48.221	1.00	31.54	T	O
ATOM	3588	N	GLU	T	62	24.146	24.042	46.060	1.00	20.11	T	N
ATOM	3589	CA	GLU	T	62	23.890	23.102	44.986	1.00	21.57	T	C
ATOM	3590	C	GLU	T	62	23.774	21.671	45.504	1.00	21.37	T	C
ATOM	3591	O	GLU	T	62	22.848	20.950	45.130	1.00	22.03	T	O
ATOM	3592	CB	GLU	T	62	24.996	23.179	43.925	1.00	20.82	T	C
ATOM	3593	CG	GLU	T	62	25.211	24.565	43.313	1.00	22.54	T	C
ATOM	3594	CD	GLU	T	62	23.923	25.198	42.794	1.00	26.23	T	C
ATOM	3595	OE1	GLU	T	62	23.135	24.492	42.164	1.00	25.97	T	O
ATOM	3596	OE2	GLU	T	62	23.717	26.403	43.012	1.00	24.60	T	O
ATOM	3597	N	ILE	T	63	24.693	21.257	46.375	1.00	19.96	T	N
ATOM	3598	CA	ILE	T	63	24.656	19.887	46.878	1.00	20.43	T	C
ATOM	3599	C	ILE	T	63	23.529	19.576	47.870	1.00	20.80	T	C
ATOM	3600	O	ILE	T	63	23.082	18.434	47.951	1.00	19.50	T	O
ATOM	3601	CB	ILE	T	63	26.035	19.460	47.477	1.00	20.40	T	C
ATOM	3602	CG1	ILE	T	63	26.424	20.356	48.654	1.00	19.56	T	C
ATOM	3603	CG2	ILE	T	63	27.105	19.513	46.398	1.00	18.09	T	C
ATOM	3604	CD1	ILE	T	63	25.877	19.894	49.986	1.00	19.85	T	C
ATOM	3605	N	VAL	T	64	23.047	20.576	48.603	1.00	20.09	T	N
ATOM	3606	CA	VAL	T	64	21.967	20.334	49.558	1.00	20.93	T	C
ATOM	3607	C	VAL	T	64	20.614	20.092	48.875	1.00	23.72	T	C
ATOM	3608	O	VAL	T	64	19.638	19.736	49.537	1.00	21.27	T	O
ATOM	3609	CB	VAL	T	64	21.804	21.501	50.568	1.00	20.02	T	C
ATOM	3610	CG1	VAL	T	64	23.093	21.690	51.358	1.00	20.46	T	C
ATOM	3611	CG2	VAL	T	64	21.405	22.775	49.842	1.00	20.60	T	C
ATOM	3612	N	LYS	T	65	20.553	20.294	47.559	1.00	25.22	T	N
ATOM	3613	CA	LYS	T	65	19.318	20.065	46.809	1.00	28.22	T	C
ATOM	3614	C	LYS	T	65	18.978	18.574	46.822	1.00	27.08	T	C
ATOM	3615	O	LYS	T	65	17.812	18.194	46.764	1.00	28.54	T	O
ATOM	3616	CB	LYS	T	65	19.466	20.565	45.366	1.00	30.57	T	C
ATOM	3617	CG	LYS	T	65	19.579	22.081	45.256	1.00	32.86	T	C
ATOM	3618	CD	LYS	T	65	19.681	22.544	43.811	1.00	35.41	T	C
ATOM	3619	CE	LYS	T	65	19.767	24.064	43.735	1.00	37.84	T	C
ATOM	3620	NZ	LYS	T	65	19.813	24.564	42.334	1.00	39.60	T	N
ATOM	3621	N	ASP	T	66	20.014	17.742	46.879	1.00	26.86	T	N
ATOM	3622	CA	ASP	T	66	19.877	16.291	46.956	1.00	24.78	T	C
ATOM	3623	C	ASP	T	66	21.205	15.780	47.494	1.00	23.00	T	C
ATOM	3624	O	ASP	T	66	22.125	15.490	46.734	1.00	21.38	T	O
ATOM	3625	CB	ASP	T	66	19.609	15.669	45.586	1.00	26.36	T	C
ATOM	3626	CG	ASP	T	66	19.251	14.188	45.680	1.00	29.40	T	C
ATOM	3627	OD1	ASP	T	66	19.538	13.568	46.722	1.00	28.55	T	O
ATOM	3628	OD2	ASP	T	66	18.695	13.648	44.717	1.00	31.14	T	O
ATOM	3629	N	VAL	T	67	21.300	15.672	48.814	1.00	22.91	T	N
ATOM	3630	CA	VAL	T	67	22.530	15.221	49.452	1.00	22.94	T	C
ATOM	3631	C	VAL	T	67	22.927	13.783	49.125	1.00	24.63	T	C

ATOM	3632	O	VAL	T	67	24.071	13.390	49.356	1.00	24.10	T	O
ATOM	3633	CB	VAL	T	67	22.449	15.384	50.992	1.00	22.47	T	C
ATOM	3634	CG1	VAL	T	67	22.180	16.846	51.350	1.00	17.69	T	C
ATOM	3635	CG2	VAL	T	67	21.364	14.488	51.563	1.00	19.93	T	C
ATOM	3636	N	LYS	T	68	21.998	13.003	48.578	1.00	26.06	T	N
ATOM	3637	CA	LYS	T	68	22.284	11.608	48.239	1.00	27.04	T	C
ATOM	3638	C	LYS	T	68	22.873	11.395	46.850	1.00	26.31	T	C
ATOM	3639	O	LYS	T	68	23.342	10.304	46.531	1.00	24.28	T	O
ATOM	3640	CB	LYS	T	68	21.024	10.759	48.401	1.00	28.46	T	C
ATOM	3641	CG	LYS	T	68	20.634	10.547	49.850	1.00	30.19	T	C
ATOM	3642	CD	LYS	T	68	19.389	9.699	49.975	1.00	32.33	T	C
ATOM	3643	CE	LYS	T	68	19.115	9.356	51.425	1.00	34.80	T	C
ATOM	3644	NZ	LYS	T	68	20.235	8.569	52.002	1.00	38.91	T	N
ATOM	3645	N	GLN	T	69	22.848	12.436	46.025	1.00	26.68	T	N
ATOM	3646	CA	GLN	T	69	23.404	12.351	44.681	1.00	24.77	T	C
ATOM	3647	C	GLN	T	69	24.924	12.389	44.739	1.00	23.29	T	C
ATOM	3648	O	GLN	T	69	25.501	12.750	45.762	1.00	22.51	T	O
ATOM	3649	CB	GLN	T	69	22.901	13.519	43.829	1.00	27.54	T	C
ATOM	3650	CG	GLN	T	69	21.556	13.274	43.173	1.00	32.96	T	C
ATOM	3651	CD	GLN	T	69	21.628	12.171	42.135	1.00	35.85	T	C
ATOM	3652	OE1	GLN	T	69	22.338	12.292	41.138	1.00	37.60	T	O
ATOM	3653	NE2	GLN	T	69	20.901	11.084	42.369	1.00	39.16	T	N
ATOM	3654	N	THR	T	70	25.562	11.995	43.640	1.00	21.11	T	N
ATOM	3655	CA	THR	T	70	27.013	12.016	43.531	1.00	20.59	T	C
ATOM	3656	C	THR	T	70	27.345	13.152	42.570	1.00	20.22	T	C
ATOM	3657	O	THR	T	70	26.917	13.149	41.414	1.00	19.62	T	O
ATOM	3658	CB	THR	T	70	27.570	10.687	42.978	1.00	19.99	T	C
ATOM	3659	OG1	THR	T	70	27.344	9.643	43.931	1.00	21.36	T	O
ATOM	3660	CG2	THR	T	70	29.067	10.802	42.728	1.00	18.95	T	C
ATOM	3661	N	TYR	T	71	28.102	14.127	43.061	1.00	18.76	T	N
ATOM	3662	CA	TYR	T	71	28.462	15.292	42.271	1.00	17.58	T	C
ATOM	3663	C	TYR	T	71	29.885	15.284	41.752	1.00	17.20	T	C
ATOM	3664	O	TYR	T	71	30.786	14.721	42.366	1.00	17.10	T	O
ATOM	3665	CB	TYR	T	71	28.263	16.572	43.095	1.00	15.82	T	C
ATOM	3666	CG	TYR	T	71	26.852	16.779	43.587	1.00	15.19	T	C
ATOM	3667	CD1	TYR	T	71	26.381	16.119	44.729	1.00	15.57	T	C
ATOM	3668	CD2	TYR	T	71	25.967	17.598	42.887	1.00	14.29	T	C
ATOM	3669	CE1	TYR	T	71	25.065	16.268	45.155	1.00	14.24	T	C
ATOM	3670	CE2	TYR	T	71	24.649	17.752	43.302	1.00	14.12	T	C
ATOM	3671	CZ	TYR	T	71	24.205	17.083	44.435	1.00	15.17	T	C
ATOM	3672	OH	TYR	T	71	22.901	17.226	44.844	1.00	13.94	T	O
ATOM	3673	N	LEU	T	72	30.077	15.926	40.609	1.00	17.96	T	N
ATOM	3674	CA	LEU	T	72	31.397	16.052	40.017	1.00	18.23	T	C
ATOM	3675	C	LEU	T	72	31.517	17.536	39.729	1.00	17.51	T	C
ATOM	3676	O	LEU	T	72	30.556	18.179	39.300	1.00	17.06	T	O
ATOM	3677	CB	LEU	T	72	31.500	15.256	38.712	1.00	22.12	T	C
ATOM	3678	CG	LEU	T	72	32.895	14.972	38.119	1.00	26.17	T	C
ATOM	3679	CD1	LEU	T	72	33.519	16.243	37.563	1.00	28.99	T	C
ATOM	3680	CD2	LEU	T	72	33.792	14.356	39.182	1.00	25.19	T	C
ATOM	3681	N	ALA	T	73	32.686	18.089	40.003	1.00	17.91	T	N
ATOM	3682	CA	ALA	T	73	32.928	19.496	39.751	1.00	16.95	T	C
ATOM	3683	C	ALA	T	73	34.197	19.592	38.922	1.00	16.12	T	C
ATOM	3684	O	ALA	T	73	34.947	18.624	38.809	1.00	18.51	T	O
ATOM	3685	CB	ALA	T	73	33.092	20.240	41.065	1.00	15.74	T	C
ATOM	3686	N	ARG	T	74	34.415	20.746	38.312	1.00	15.02	T	N
ATOM	3687	CA	ARG	T	74	35.613	20.966	37.524	1.00	14.43	T	C

ATOM	3688	C	ARG	T	74	35.926	22.453	37.535	1.00	14.10	T	C
ATOM	3689	O	ARG	T	74	35.024	23.293	37.512	1.00	13.27	T	O
ATOM	3690	CB	ARG	T	74	35.444	20.438	36.090	1.00	13.57	T	C
ATOM	3691	CG	ARG	T	74	34.246	20.959	35.312	1.00	15.95	T	C
ATOM	3692	CD	ARG	T	74	34.070	20.161	34.015	1.00	15.26	T	C
ATOM	3693	NE	ARG	T	74	32.983	20.658	33.173	1.00	11.15	T	N
ATOM	3694	CZ	ARG	T	74	32.545	20.051	32.071	1.00	13.10	T	C
ATOM	3695	NH1	ARG	T	74	33.093	18.910	31.661	1.00	9.53	T	N
ATOM	3696	NH2	ARG	T	74	31.562	20.594	31.364	1.00	10.82	T	N
ATOM	3697	N	VAL	T	75	37.211	22.757	37.599	1.00	14.14	T	N
ATOM	3698	CA	VAL	T	75	37.672	24.147	37.643	1.00	15.10	T	C
ATOM	3699	C	VAL	T	75	38.307	24.589	36.333	1.00	16.01	T	C
ATOM	3700	O	VAL	T	75	39.301	24.016	35.896	1.00	14.34	T	O
ATOM	3701	CB	VAL	T	75	38.708	24.336	38.773	1.00	15.28	T	C
ATOM	3702	CG1	VAL	T	75	39.280	25.747	38.731	1.00	13.98	T	C
ATOM	3703	CG2	VAL	T	75	38.058	24.065	40.122	1.00	14.39	T	C
ATOM	3704	N	PHE	T	76	37.722	25.604	35.708	1.00	18.72	T	N
ATOM	3705	CA	PHE	T	76	38.247	26.140	34.460	1.00	21.14	T	C
ATOM	3706	C	PHE	T	76	39.211	27.272	34.780	1.00	22.66	T	C
ATOM	3707	O	PHE	T	76	38.992	28.035	35.723	1.00	23.68	T	O
ATOM	3708	CB	PHE	T	76	37.112	26.668	33.583	1.00	23.60	T	C
ATOM	3709	CG	PHE	T	76	36.199	25.596	33.062	1.00	28.84	T	C
ATOM	3710	CD1	PHE	T	76	36.660	24.654	32.152	1.00	31.44	T	C
ATOM	3711	CD2	PHE	T	76	34.880	25.521	33.486	1.00	31.69	T	C
ATOM	3712	CE1	PHE	T	76	35.818	23.652	31.671	1.00	33.34	T	C
ATOM	3713	CE2	PHE	T	76	34.034	24.522	33.008	1.00	34.41	T	C
ATOM	3714	CZ	PHE	T	76	34.505	23.589	32.101	1.00	30.45	T	C
ATOM	3715	N	SER	T	77	40.282	27.369	34.000	1.00	24.37	T	N
ATOM	3716	CA	SER	T	77	41.287	28.410	34.182	1.00	25.59	T	C
ATOM	3717	C	SER	T	77	41.337	29.303	32.953	1.00	27.03	T	C
ATOM	3718	O	SER	T	77	41.322	28.817	31.823	1.00	25.41	T	O
ATOM	3719	CB	SER	T	77	42.668	27.793	34.401	1.00	26.08	T	C
ATOM	3720	OG	SER	T	77	42.714	27.056	35.604	1.00	28.24	T	O
ATOM	3721	N	TYR	T	78	41.398	30.610	33.188	1.00	29.89	T	N
ATOM	3722	CA	TYR	T	78	41.465	31.601	32.119	1.00	31.65	T	C
ATOM	3723	C	TYR	T	78	42.636	32.537	32.414	1.00	33.58	T	C
ATOM	3724	O	TYR	T	78	43.009	32.726	33.572	1.00	34.76	T	O
ATOM	3725	CB	TYR	T	78	40.173	32.413	32.073	1.00	31.59	T	C
ATOM	3726	CG	TYR	T	78	38.919	31.579	31.943	1.00	31.52	T	C
ATOM	3727	CD1	TYR	T	78	38.505	31.093	30.706	1.00	29.66	T	C
ATOM	3728	CD2	TYR	T	78	38.147	31.274	33.062	1.00	30.05	T	C
ATOM	3729	CE1	TYR	T	78	37.352	30.331	30.587	1.00	30.62	T	C
ATOM	3730	CE2	TYR	T	78	36.998	30.512	32.955	1.00	30.31	T	C
ATOM	3731	CZ	TYR	T	78	36.604	30.044	31.716	1.00	30.37	T	C
ATOM	3732	OH	TYR	T	78	35.458	29.296	31.607	1.00	31.28	T	O
ATOM	3733	N	PRO	T	79	43.236	33.132	31.372	1.00	35.05	T	N
ATOM	3734	CA	PRO	T	79	44.365	34.047	31.573	1.00	35.74	T	C
ATOM	3735	C	PRO	T	79	43.914	35.395	32.139	1.00	36.81	T	C
ATOM	3736	O	PRO	T	79	43.932	35.611	33.352	1.00	37.66	T	O
ATOM	3737	CB	PRO	T	79	44.949	34.178	30.173	1.00	35.23	T	C
ATOM	3738	CG	PRO	T	79	43.723	34.105	29.313	1.00	35.61	T	C
ATOM	3739	CD	PRO	T	79	42.960	32.951	29.935	1.00	35.09	T	C
ATOM	3740	N	GLU	T	91	38.161	24.891	23.662	1.00	26.53	T	N
ATOM	3741	CA	GLU	T	91	37.694	24.757	25.073	1.00	26.00	T	C
ATOM	3742	C	GLU	T	91	38.810	25.160	26.043	1.00	26.45	T	C
ATOM	3743	O	GLU	T	91	39.991	24.986	25.748	1.00	24.05	T	O

ATOM	3744	CB	GLU	T	91	37.238	23.315	25.331	1.00	24.69	T	C
ATOM	3745	CG	GLU	T	91	36.117	22.857	24.384	1.00	22.94	T	C
ATOM	3746	CD	GLU	T	91	35.711	21.405	24.588	1.00	20.53	T	C
ATOM	3747	OE1	GLU	T	91	36.581	20.582	24.780	1.00	21.42	T	O
ATOM	3748	OE2	GLU	T	91	34.525	21.111	24.538	1.00	21.55	T	O
ATOM	3749	N	PRO	T	92	38.443	25.714	27.212	1.00	27.49	T	N
ATOM	3750	CA	PRO	T	92	39.402	26.153	28.232	1.00	28.13	T	C
ATOM	3751	C	PRO	T	92	40.087	25.028	28.998	1.00	27.90	T	C
ATOM	3752	O	PRO	T	92	39.618	23.893	29.012	1.00	28.67	T	O
ATOM	3753	CB	PRO	T	92	38.545	27.016	29.148	1.00	29.05	T	C
ATOM	3754	CG	PRO	T	92	37.243	26.282	29.135	1.00	30.13	T	C
ATOM	3755	CD	PRO	T	92	37.063	25.993	27.650	1.00	28.84	T	C
ATOM	3756	N	LEU	T	93	41.199	25.361	29.642	1.00	28.40	T	N
ATOM	3757	CA	LEU	T	93	41.944	24.392	30.435	1.00	27.14	T	C
ATOM	3758	C	LEU	T	93	41.152	24.159	31.710	1.00	24.86	T	C
ATOM	3759	O	LEU	T	93	40.576	25.094	32.268	1.00	23.66	T	O
ATOM	3760	CB	LEU	T	93	43.327	24.936	30.797	1.00	29.29	T	C
ATOM	3761	CG	LEU	T	93	44.208	25.476	29.665	1.00	33.20	T	C
ATOM	3762	CD1	LEU	T	93	45.541	25.928	30.247	1.00	34.70	T	C
ATOM	3763	CD2	LEU	T	93	44.426	24.412	28.604	1.00	34.85	T	C
ATOM	3764	N	TYR	T	94	41.108	22.912	32.162	1.00	23.07	T	N
ATOM	3765	CA	TYR	T	94	40.379	22.584	33.379	1.00	20.97	T	C
ATOM	3766	C	TYR	T	94	40.878	21.296	34.007	1.00	19.78	T	C
ATOM	3767	O	TYR	T	94	41.676	20.562	33.422	1.00	18.62	T	O
ATOM	3768	CB	TYR	T	94	38.875	22.454	33.104	1.00	20.47	T	C
ATOM	3769	CG	TYR	T	94	38.496	21.246	32.272	1.00	21.39	T	C
ATOM	3770	CD1	TYR	T	94	38.595	21.268	30.877	1.00	20.22	T	C
ATOM	3771	CD2	TYR	T	94	38.054	20.071	32.883	1.00	19.95	T	C
ATOM	3772	CE1	TYR	T	94	38.266	20.149	30.113	1.00	20.60	T	C
ATOM	3773	CE2	TYR	T	94	37.719	18.947	32.128	1.00	20.65	T	C
ATOM	3774	CZ	TYR	T	94	37.828	18.993	30.747	1.00	21.30	T	C
ATOM	3775	OH	TYR	T	94	37.508	17.881	30.004	1.00	21.41	T	O
ATOM	3776	N	GLU	T	95	40.380	21.035	35.207	1.00	18.35	T	N
ATOM	3777	CA	GLU	T	95	40.733	19.857	35.976	1.00	19.30	T	C
ATOM	3778	C	GLU	T	95	39.452	19.393	36.660	1.00	18.34	T	C
ATOM	3779	O	GLU	T	95	38.667	20.216	37.133	1.00	17.95	T	O
ATOM	3780	CB	GLU	T	95	41.782	20.231	37.028	1.00	22.02	T	C
ATOM	3781	CG	GLU	T	95	42.241	19.097	37.936	1.00	28.22	T	C
ATOM	3782	CD	GLU	T	95	43.004	18.024	37.189	1.00	30.84	T	C
ATOM	3783	OE1	GLU	T	95	43.404	18.269	36.044	1.00	34.07	T	O
ATOM	3784	OE2	GLU	T	95	43.205	16.957	37.753	1.00	31.49	T	O
ATOM	3785	N	ASN	T	96	39.233	18.084	36.697	1.00	15.73	T	N
ATOM	3786	CA	ASN	T	96	38.052	17.537	37.348	1.00	16.84	T	C
ATOM	3787	C	ASN	T	96	38.375	17.281	38.815	1.00	16.63	T	C
ATOM	3788	O	ASN	T	96	39.526	17.045	39.172	1.00	17.38	T	O
ATOM	3789	CB	ASN	T	96	37.623	16.211	36.703	1.00	15.17	T	C
ATOM	3790	CG	ASN	T	96	37.110	16.381	35.279	1.00	18.47	T	C
ATOM	3791	OD1	ASN	T	96	36.458	17.371	34.957	1.00	16.54	T	O
ATOM	3792	ND2	ASN	T	96	37.384	15.394	34.425	1.00	16.63	T	N
ATOM	3793	N	SER	T	97	37.355	17.335	39.660	1.00	15.24	T	N
ATOM	3794	CA	SER	T	97	37.523	17.068	41.082	1.00	17.45	T	C
ATOM	3795	C	SER	T	97	37.125	15.613	41.313	1.00	18.06	T	C
ATOM	3796	O	SER	T	97	36.594	14.958	40.419	1.00	18.60	T	O
ATOM	3797	CB	SER	T	97	36.575	17.935	41.893	1.00	16.21	T	C
ATOM	3798	OG	SER	T	97	35.238	17.519	41.660	1.00	15.25	T	O
ATOM	3799	N	PRO	T	98	37.402	15.076	42.508	1.00	19.40	T	N

ATOM	3800	CA	PRO	T	98	36.991	13.686	42.710	1.00	19.93	T	C
ATOM	3801	C	PRO	T	98	35.478	13.714	42.878	1.00	19.53	T	C
ATOM	3802	O	PRO	T	98	34.907	14.767	43.139	1.00	20.13	T	O
ATOM	3803	CB	PRO	T	98	37.716	13.289	43.997	1.00	22.25	T	C
ATOM	3804	CG	PRO	T	98	37.885	14.595	44.720	1.00	22.51	T	C
ATOM	3805	CD	PRO	T	98	38.269	15.537	43.606	1.00	21.73	T	C
ATOM	3806	N	GLU	T	99	34.819	12.579	42.708	1.00	19.80	T	N
ATOM	3807	CA	GLU	T	99	33.378	12.555	42.872	1.00	20.54	T	C
ATOM	3808	C	GLU	T	99	33.076	12.827	44.334	1.00	20.49	T	C
ATOM	3809	O	GLU	T	99	33.882	12.511	45.210	1.00	20.71	T	O
ATOM	3810	CB	GLU	T	99	32.819	11.198	42.464	1.00	23.90	T	C
ATOM	3811	CG	GLU	T	99	33.062	10.850	41.009	1.00	30.24	T	C
ATOM	3812	CD	GLU	T	99	32.382	9.561	40.609	1.00	34.08	T	C
ATOM	3813	OE1	GLU	T	99	32.625	8.547	41.256	1.00	39.49	T	O
ATOM	3814	OE2	GLU	T	99	31.619	9.578	39.661	1.00	37.57	T	O
ATOM	3815	N	PHE	T	100	31.921	13.422	44.603	1.00	19.39	T	N
ATOM	3816	CA	PHE	T	100	31.552	13.723	45.974	1.00	20.04	T	C
ATOM	3817	C	PHE	T	100	30.099	13.404	46.279	1.00	19.86	T	C
ATOM	3818	O	PHE	T	100	29.195	13.977	45.684	1.00	22.07	T	O
ATOM	3819	CB	PHE	T	100	31.810	15.202	46.285	1.00	18.94	T	C
ATOM	3820	CG	PHE	T	100	31.554	15.570	47.721	1.00	17.26	T	C
ATOM	3821	CD1	PHE	T	100	32.348	15.051	48.734	1.00	17.16	T	C
ATOM	3822	CD2	PHE	T	100	30.506	16.417	48.063	1.00	17.80	T	C
ATOM	3823	CE1	PHE	T	100	32.102	15.369	50.072	1.00	18.82	T	C
ATOM	3824	CE2	PHE	T	100	30.252	16.739	49.402	1.00	18.00	T	C
ATOM	3825	CZ	PHE	T	100	31.053	16.212	50.405	1.00	14.11	T	C
ATOM	3826	N	THR	T	101	29.880	12.486	47.213	1.00	19.96	T	N
ATOM	3827	CA	THR	T	101	28.529	12.125	47.618	1.00	19.19	T	C
ATOM	3828	C	THR	T	101	28.359	12.669	49.032	1.00	19.73	T	C
ATOM	3829	O	THR	T	101	28.774	12.041	50.005	1.00	19.00	T	O
ATOM	3830	CB	THR	T	101	28.339	10.602	47.616	1.00	19.88	T	C
ATOM	3831	OG1	THR	T	101	28.767	10.075	46.353	1.00	19.78	T	O
ATOM	3832	CG2	THR	T	101	26.869	10.252	47.842	1.00	16.06	T	C
ATOM	3833	N	PRO	T	102	27.740	13.851	49.159	1.00	20.90	T	N
ATOM	3834	CA	PRO	T	102	27.512	14.514	50.450	1.00	20.65	T	C
ATOM	3835	C	PRO	T	102	27.112	13.595	51.599	1.00	21.85	T	C
ATOM	3836	O	PRO	T	102	27.826	13.483	52.594	1.00	22.55	T	O
ATOM	3837	CB	PRO	T	102	26.426	15.539	50.126	1.00	20.56	T	C
ATOM	3838	CG	PRO	T	102	26.710	15.892	48.691	1.00	19.84	T	C
ATOM	3839	CD	PRO	T	102	27.008	14.540	48.079	1.00	20.33	T	C
ATOM	3840	N	TYR	T	103	25.964	12.946	51.458	1.00	21.87	T	N
ATOM	3841	CA	TYR	T	103	25.441	12.050	52.484	1.00	22.45	T	C
ATOM	3842	C	TYR	T	103	26.464	11.034	53.003	1.00	22.95	T	C
ATOM	3843	O	TYR	T	103	26.534	10.774	54.200	1.00	23.24	T	O
ATOM	3844	CB	TYR	T	103	24.222	11.308	51.936	1.00	23.18	T	C
ATOM	3845	CG	TYR	T	103	23.404	10.588	52.983	1.00	23.57	T	C
ATOM	3846	CD1	TYR	T	103	22.458	11.272	53.747	1.00	23.47	T	C
ATOM	3847	CD2	TYR	T	103	23.559	9.220	53.197	1.00	22.61	T	C
ATOM	3848	CE1	TYR	T	103	21.684	10.612	54.693	1.00	23.51	T	C
ATOM	3849	CE2	TYR	T	103	22.785	8.548	54.145	1.00	23.64	T	C
ATOM	3850	CZ	TYR	T	103	21.852	9.251	54.885	1.00	23.20	T	C
ATOM	3851	OH	TYR	T	103	21.089	8.602	55.824	1.00	24.87	T	O
ATOM	3852	N	LEU	T	104	27.256	10.465	52.101	1.00	23.67	T	N
ATOM	3853	CA	LEU	T	104	28.250	9.468	52.474	1.00	22.89	T	C
ATOM	3854	C	LEU	T	104	29.579	10.006	53.000	1.00	23.88	T	C
ATOM	3855	O	LEU	T	104	30.272	9.307	53.743	1.00	23.44	T	O

ATOM	3856	CB	LEU	T	104	28.546	8.550	51.285	1.00	22.13	T	C
ATOM	3857	CG	LEU	T	104	27.414	7.715	50.680	1.00	23.01	T	C
ATOM	3858	CD1	LEU	T	104	27.973	6.885	49.531	1.00	20.25	T	C
ATOM	3859	CD2	LEU	T	104	26.797	6.808	51.747	1.00	20.91	T	C
ATOM	3860	N	GLU	T	105	29.957	11.225	52.627	1.00	23.91	T	N
ATOM	3861	CA	GLU	T	105	31.243	11.733	53.092	1.00	25.61	T	C
ATOM	3862	C	GLU	T	105	31.364	13.110	53.752	1.00	24.53	T	C
ATOM	3863	O	GLU	T	105	32.473	13.529	54.080	1.00	24.54	T	O
ATOM	3864	CB	GLU	T	105	32.281	11.599	51.967	1.00	26.37	T	C
ATOM	3865	CG	GLU	T	105	31.867	12.121	50.611	1.00	28.41	T	C
ATOM	3866	CD	GLU	T	105	32.602	11.421	49.471	1.00	27.99	T	C
ATOM	3867	OE1	GLU	T	105	33.821	11.326	49.516	1.00	27.95	T	O
ATOM	3868	OE2	GLU	T	105	31.950	10.979	48.543	1.00	27.09	T	O
ATOM	3869	N	THR	T	106	30.258	13.813	53.973	1.00	23.46	T	N
ATOM	3870	CA	THR	T	106	30.367	15.112	54.632	1.00	22.92	T	C
ATOM	3871	C	THR	T	106	30.738	14.856	56.091	1.00	24.04	T	C
ATOM	3872	O	THR	T	106	30.143	14.002	56.752	1.00	22.58	T	O
ATOM	3873	CB	THR	T	106	29.052	15.919	54.586	1.00	21.63	T	C
ATOM	3874	OG1	THR	T	106	29.308	17.265	55.010	1.00	21.19	T	O
ATOM	3875	CG2	THR	T	106	28.009	15.312	55.506	1.00	21.52	T	C
ATOM	3876	N	ASN	T	107	31.728	15.587	56.588	1.00	22.90	T	N
ATOM	3877	CA	ASN	T	107	32.171	15.417	57.965	1.00	24.07	T	C
ATOM	3878	C	ASN	T	107	31.108	15.795	58.978	1.00	24.33	T	C
ATOM	3879	O	ASN	T	107	30.380	16.773	58.799	1.00	24.71	T	O
ATOM	3880	CB	ASN	T	107	33.424	16.252	58.232	1.00	24.30	T	C
ATOM	3881	CG	ASN	T	107	34.633	15.725	57.507	1.00	25.25	T	C
ATOM	3882	OD1	ASN	T	107	35.037	14.582	57.707	1.00	29.41	T	O
ATOM	3883	ND2	ASN	T	107	35.223	16.553	56.657	1.00	28.39	T	N
ATOM	3884	N	LEU	T	108	31.017	15.006	60.041	1.00	24.30	T	N
ATOM	3885	CA	LEU	T	108	30.068	15.279	61.110	1.00	24.22	T	C
ATOM	3886	C	LEU	T	108	30.744	16.309	62.007	1.00	22.82	T	C
ATOM	3887	O	LEU	T	108	31.870	16.105	62.452	1.00	21.51	T	O
ATOM	3888	CB	LEU	T	108	29.772	13.998	61.890	1.00	25.35	T	C
ATOM	3889	CG	LEU	T	108	29.094	12.904	61.062	1.00	27.74	T	C
ATOM	3890	CD1	LEU	T	108	29.156	11.562	61.786	1.00	27.60	T	C
ATOM	3891	CD2	LEU	T	108	27.659	13.318	60.786	1.00	28.49	T	C
ATOM	3892	N	GLY	T	109	30.066	17.425	62.252	1.00	23.68	T	N
ATOM	3893	CA	GLY	T	109	30.648	18.461	63.084	1.00	22.92	T	C
ATOM	3894	C	GLY	T	109	30.829	18.004	64.520	1.00	23.12	T	C
ATOM	3895	O	GLY	T	109	30.240	17.003	64.927	1.00	21.62	T	O
ATOM	3896	N	GLN	T	110	31.656	18.718	65.281	1.00	21.54	T	N
ATOM	3897	CA	GLN	T	110	31.869	18.378	66.683	1.00	21.94	T	C
ATOM	3898	C	GLN	T	110	30.527	18.570	67.381	1.00	21.65	T	C
ATOM	3899	O	GLN	T	110	29.916	19.630	67.276	1.00	21.94	T	O
ATOM	3900	CB	GLN	T	110	32.919	19.304	67.313	1.00	21.36	T	C
ATOM	3901	CG	GLN	T	110	33.166	19.045	68.802	1.00	21.01	T	C
ATOM	3902	CD	GLN	T	110	34.203	19.979	69.398	1.00	21.94	T	C
ATOM	3903	OE1	GLN	T	110	34.139	21.189	69.207	1.00	24.10	T	O
ATOM	3904	NE2	GLN	T	110	35.162	19.419	70.132	1.00	21.56	T	N
ATOM	3905	N	PRO	T	111	30.045	17.542	68.094	1.00	23.09	T	N
ATOM	3906	CA	PRO	T	111	28.762	17.651	68.790	1.00	22.88	T	C
ATOM	3907	C	PRO	T	111	28.920	18.496	70.043	1.00	24.37	T	C
ATOM	3908	O	PRO	T	111	30.032	18.876	70.408	1.00	24.44	T	O
ATOM	3909	CB	PRO	T	111	28.418	16.198	69.141	1.00	23.56	T	C
ATOM	3910	CG	PRO	T	111	29.425	15.358	68.352	1.00	23.39	T	C
ATOM	3911	CD	PRO	T	111	30.641	16.217	68.322	1.00	22.94	T	C

ATOM	3912	N	THR	T	112	27.797	18.769	70.697	1.00	25.07	T	N
ATOM	3913	CA	THR	T	112	27.762	19.552	71.918	1.00	25.43	T	C
ATOM	3914	C	THR	T	112	26.764	18.915	72.880	1.00	26.70	T	C
ATOM	3915	O	THR	T	112	25.616	18.681	72.512	1.00	26.69	T	O
ATOM	3916	CB	THR	T	112	27.295	21.001	71.645	1.00	27.11	T	C
ATOM	3917	OG1	THR	T	112	28.261	21.673	70.830	1.00	29.22	T	O
ATOM	3918	CG2	THR	T	112	27.114	21.765	72.955	1.00	26.39	T	C
ATOM	3919	N	ILE	T	113	27.202	18.626	74.102	1.00	26.55	T	N
ATOM	3920	CA	ILE	T	113	26.314	18.057	75.111	1.00	27.02	T	C
ATOM	3921	C	ILE	T	113	25.371	19.181	75.536	1.00	28.66	T	C
ATOM	3922	O	ILE	T	113	25.811	20.228	76.010	1.00	29.26	T	O
ATOM	3923	CB	ILE	T	113	27.117	17.541	76.337	1.00	26.73	T	C
ATOM	3924	CG1	ILE	T	113	27.926	16.305	75.935	1.00	24.38	T	C
ATOM	3925	CG2	ILE	T	113	26.179	17.208	77.490	1.00	25.10	T	C
ATOM	3926	CD1	ILE	T	113	28.821	15.766	77.021	1.00	27.02	T	C
ATOM	3927	N	GLN	T	114	24.073	18.967	75.347	1.00	30.54	T	N
ATOM	3928	CA	GLN	T	114	23.069	19.967	75.690	1.00	31.98	T	C
ATOM	3929	C	GLN	T	114	22.772	20.033	77.185	1.00	33.02	T	C
ATOM	3930	O	GLN	T	114	22.588	21.119	77.739	1.00	33.20	T	O
ATOM	3931	CB	GLN	T	114	21.773	19.688	74.926	1.00	32.72	T	C
ATOM	3932	CG	GLN	T	114	20.714	20.773	75.070	1.00	34.48	T	C
ATOM	3933	CD	GLN	T	114	19.499	20.516	74.199	1.00	36.97	T	C
ATOM	3934	OE1	GLN	T	114	18.648	19.686	74.523	1.00	39.79	T	O
ATOM	3935	NE2	GLN	T	114	19.421	21.218	73.077	1.00	37.84	T	N
ATOM	3936	N	SER	T	115	22.721	18.873	77.833	1.00	34.02	T	N
ATOM	3937	CA	SER	T	115	22.442	18.810	79.262	1.00	34.71	T	C
ATOM	3938	C	SER	T	115	22.528	17.392	79.811	1.00	36.31	T	C
ATOM	3939	O	SER	T	115	22.729	16.429	79.072	1.00	34.54	T	O
ATOM	3940	CB	SER	T	115	21.041	19.350	79.544	1.00	34.16	T	C
ATOM	3941	OG	SER	T	115	20.056	18.493	78.989	1.00	34.47	T	O
ATOM	3942	N	PHE	T	116	22.384	17.286	81.126	1.00	39.39	T	N
ATOM	3943	CA	PHE	T	116	22.391	16.006	81.814	1.00	43.50	T	C
ATOM	3944	C	PHE	T	116	21.700	16.155	83.160	1.00	45.33	T	C
ATOM	3945	O	PHE	T	116	22.130	16.930	84.013	1.00	46.10	T	O
ATOM	3946	CB	PHE	T	116	23.816	15.449	81.990	1.00	43.81	T	C
ATOM	3947	CG	PHE	T	116	24.829	16.456	82.449	1.00	44.31	T	C
ATOM	3948	CD1	PHE	T	116	25.669	17.079	81.532	1.00	46.06	T	C
ATOM	3949	CD2	PHE	T	116	24.976	16.753	83.797	1.00	45.66	T	C
ATOM	3950	CE1	PHE	T	116	26.643	17.977	81.949	1.00	45.84	T	C
ATOM	3951	CE2	PHE	T	116	25.946	17.651	84.227	1.00	46.21	T	C
ATOM	3952	CZ	PHE	T	116	26.783	18.264	83.299	1.00	47.39	T	C
ATOM	3953	N	GLU	T	117	20.609	15.416	83.331	1.00	47.44	T	N
ATOM	3954	CA	GLU	T	117	19.832	15.465	84.561	1.00	50.33	T	C
ATOM	3955	C	GLU	T	117	19.909	14.160	85.340	1.00	51.09	T	C
ATOM	3956	O	GLU	T	117	19.858	13.073	84.765	1.00	50.21	T	O
ATOM	3957	CB	GLU	T	117	18.368	15.770	84.239	1.00	52.68	T	C
ATOM	3958	CG	GLU	T	117	17.499	16.012	85.462	1.00	54.67	T	C
ATOM	3959	CD	GLU	T	117	16.035	16.159	85.114	1.00	56.19	T	C
ATOM	3960	OE1	GLU	T	117	15.263	16.548	85.987	1.00	58.48	T	O
ATOM	3961	OE2	GLU	T	117	15.671	15.878	83.971	1.00	57.72	T	O
ATOM	3962	N	GLN	T	118	20.026	14.278	86.657	1.00	52.53	T	N
ATOM	3963	CA	GLN	T	118	20.091	13.113	87.524	1.00	53.52	T	C
ATOM	3964	C	GLN	T	118	18.790	12.987	88.307	1.00	53.74	T	C
ATOM	3965	O	GLN	T	118	18.292	13.967	88.863	1.00	52.43	T	O
ATOM	3966	CB	GLN	T	118	21.268	13.237	88.495	1.00	55.69	T	C
ATOM	3967	CG	GLN	T	118	21.248	14.505	89.345	1.00	58.28	T	C

ATOM	3968	CD	GLN	T	118	22.398	14.581	90.341	1.00	59.98	T C
ATOM	3969	OE1	GLN	T	118	22.559	15.585	91.038	1.00	60.49	T O
ATOM	3970	NE2	GLN	T	118	23.198	13.520	90.417	1.00	59.89	T N
ATOM	3971	N	VAL	T	119	18.236	11.780	88.336	1.00	54.32	T N
ATOM	3972	CA	VAL	T	119	16.999	11.527	89.064	1.00	55.20	T C
ATOM	3973	C	VAL	T	119	17.342	10.874	90.400	1.00	55.28	T C
ATOM	3974	O	VAL	T	119	17.050	11.421	91.465	1.00	55.61	T O
ATOM	3975	CB	VAL	T	119	16.056	10.592	88.270	1.00	55.27	T C
ATOM	3976	CG1	VAL	T	119	14.808	10.294	89.089	1.00	55.95	T C
ATOM	3977	CG2	VAL	T	119	15.675	11.239	86.948	1.00	55.25	T C
ATOM	3978	N	GLY	T	120	17.968	9.705	90.330	1.00	54.96	T N
ATOM	3979	CA	GLY	T	120	18.357	8.992	91.531	1.00	55.01	T C
ATOM	3980	C	GLY	T	120	19.681	8.294	91.305	1.00	55.06	T C
ATOM	3981	O	GLY	T	120	20.739	8.802	91.681	1.00	54.95	T O
ATOM	3982	N	THR	T	121	19.622	7.124	90.680	1.00	54.66	T N
ATOM	3983	CA	THR	T	121	20.824	6.356	90.388	1.00	54.74	T C
ATOM	3984	C	THR	T	121	21.039	6.232	88.876	1.00	53.59	T C
ATOM	3985	O	THR	T	121	21.706	5.311	88.406	1.00	53.56	T O
ATOM	3986	CB	THR	T	121	20.743	4.945	91.010	1.00	55.32	T C
ATOM	3987	OG1	THR	T	121	21.985	4.259	90.805	1.00	56.26	T O
ATOM	3988	CG2	THR	T	121	19.607	4.145	90.379	1.00	55.25	T C
ATOM	3989	N	LYS	T	122	20.474	7.171	88.122	1.00	52.48	T N
ATOM	3990	CA	LYS	T	122	20.599	7.178	86.669	1.00	51.79	T C
ATOM	3991	C	LYS	T	122	20.720	8.611	86.155	1.00	50.74	T C
ATOM	3992	O	LYS	T	122	20.121	9.532	86.713	1.00	50.69	T O
ATOM	3993	CB	LYS	T	122	19.385	6.493	86.038	1.00	52.21	T C
ATOM	3994	CG	LYS	T	122	19.206	5.042	86.475	1.00	53.53	T C
ATOM	3995	CD	LYS	T	122	17.813	4.797	87.036	1.00	55.85	T C
ATOM	3996	CE	LYS	T	122	17.508	5.721	88.216	1.00	57.36	T C
ATOM	3997	NZ	LYS	T	122	16.108	5.599	88.713	1.00	55.80	T N
ATOM	3998	N	VAL	T	123	21.498	8.792	85.091	1.00	48.62	T N
ATOM	3999	CA	VAL	T	123	21.712	10.111	84.504	1.00	46.58	T C
ATOM	4000	C	VAL	T	123	21.280	10.170	83.040	1.00	44.65	T C
ATOM	4001	O	VAL	T	123	21.533	9.248	82.267	1.00	45.12	T O
ATOM	4002	CB	VAL	T	123	23.207	10.519	84.597	1.00	46.69	T C
ATOM	4003	CG1	VAL	T	123	23.439	11.859	83.907	1.00	46.11	T C
ATOM	4004	CG2	VAL	T	123	23.630	10.599	86.055	1.00	46.67	T C
ATOM	4005	N	ASN	T	124	20.622	11.261	82.670	1.00	42.65	T N
ATOM	4006	CA	ASN	T	124	20.171	11.456	81.301	1.00	41.30	T C
ATOM	4007	C	ASN	T	124	21.069	12.470	80.604	1.00	38.83	T C
ATOM	4008	O	ASN	T	124	21.026	13.655	80.915	1.00	38.66	T O
ATOM	4009	CB	ASN	T	124	18.725	11.957	81.282	1.00	42.92	T C
ATOM	4010	CG	ASN	T	124	18.287	12.420	79.904	1.00	45.20	T C
ATOM	4011	OD1	ASN	T	124	18.444	11.703	78.917	1.00	47.86	T O
ATOM	4012	ND2	ASN	T	124	17.728	13.623	79.833	1.00	46.71	T N
ATOM	4013	N	VAL	T	125	21.892	11.999	79.674	1.00	35.58	T N
ATOM	4014	CA	VAL	T	125	22.779	12.890	78.934	1.00	34.22	T C
ATOM	4015	C	VAL	T	125	22.150	13.178	77.576	1.00	32.94	T C
ATOM	4016	O	VAL	T	125	21.938	12.273	76.776	1.00	32.50	T O
ATOM	4017	CB	VAL	T	125	24.180	12.264	78.723	1.00	33.64	T C
ATOM	4018	CG1	VAL	T	125	25.051	13.205	77.897	1.00	33.24	T C
ATOM	4019	CG2	VAL	T	125	24.840	11.994	80.069	1.00	31.46	T C
ATOM	4020	N	THR	T	126	21.835	14.442	77.332	1.00	31.93	T N
ATOM	4021	CA	THR	T	126	21.225	14.847	76.078	1.00	31.44	T C
ATOM	4022	C	THR	T	126	22.246	15.541	75.181	1.00	30.53	T C
ATOM	4023	O	THR	T	126	22.995	16.406	75.631	1.00	30.92	T O

ATOM	4024	CB	THR	T	126	20.035	15.801	76.333	1.00	32.80	T	C
ATOM	4025	OG1	THR	T	126	19.046	15.126	77.123	1.00	34.45	T	O
ATOM	4026	CG2	THR	T	126	19.404	16.248	75.018	1.00	33.11	T	C
ATOM	4027	N	VAL	T	127	22.273	15.144	73.915	1.00	28.54	T	N
ATOM	4028	CA	VAL	T	127	23.181	15.720	72.931	1.00	28.68	T	C
ATOM	4029	C	VAL	T	127	22.381	16.700	72.074	1.00	29.29	T	C
ATOM	4030	O	VAL	T	127	21.293	16.376	71.596	1.00	28.57	T	O
ATOM	4031	CB	VAL	T	127	23.776	14.631	72.009	1.00	27.25	T	C
ATOM	4032	CG1	VAL	T	127	24.740	15.260	71.013	1.00	28.11	T	C
ATOM	4033	CG2	VAL	T	127	24.478	13.567	72.837	1.00	26.10	T	C
ATOM	4034	N	GLU	T	128	22.923	17.896	71.880	1.00	30.12	T	N
ATOM	4035	CA	GLU	T	128	22.248	18.920	71.094	1.00	32.79	T	C
ATOM	4036	C	GLU	T	128	22.060	18.489	69.642	1.00	33.25	T	C
ATOM	4037	O	GLU	T	128	23.005	18.051	68.987	1.00	32.52	T	O
ATOM	4038	CB	GLU	T	128	23.049	20.222	71.146	1.00	35.07	T	C
ATOM	4039	CG	GLU	T	128	22.327	21.419	70.558	1.00	39.25	T	C
ATOM	4040	CD	GLU	T	128	23.162	22.681	70.624	1.00	42.60	T	C
ATOM	4041	OE1	GLU	T	128	24.132	22.785	69.872	1.00	42.38	T	O
ATOM	4042	OE2	GLU	T	128	22.842	23.549	71.436	1.00	44.49	T	O
ATOM	4043	N	ASP	T	129	20.834	18.602	69.146	1.00	34.87	T	N
ATOM	4044	CA	ASP	T	129	20.543	18.234	67.765	1.00	38.67	T	C
ATOM	4045	C	ASP	T	129	21.016	19.404	66.908	1.00	39.15	T	C
ATOM	4046	O	ASP	T	129	20.271	20.355	66.684	1.00	40.95	T	O
ATOM	4047	CB	ASP	T	129	19.038	18.020	67.571	1.00	41.05	T	C
ATOM	4048	CG	ASP	T	129	18.721	17.167	66.354	1.00	44.26	T	C
ATOM	4049	OD1	ASP	T	129	19.421	17.291	65.355	1.00	45.06	T	O
ATOM	4050	OD2	ASP	T	129	17.768	16.387	66.411	1.00	46.55	T	O
ATOM	4051	N	GLU	T	130	22.259	19.328	66.442	1.00	39.21	T	N
ATOM	4052	CA	GLU	T	130	22.859	20.388	65.639	1.00	39.23	T	C
ATOM	4053	C	GLU	T	130	22.242	20.531	64.257	1.00	37.36	T	C
ATOM	4054	O	GLU	T	130	21.867	19.548	63.627	1.00	35.82	T	O
ATOM	4055	CB	GLU	T	130	24.362	20.145	65.485	1.00	43.16	T	C
ATOM	4056	CG	GLU	T	130	25.175	21.419	65.294	1.00	46.75	T	C
ATOM	4057	CD	GLU	T	130	26.607	21.139	64.891	1.00	48.44	T	C
ATOM	4058	OE1	GLU	T	130	26.819	20.722	63.766	1.00	52.82	T	O
ATOM	4059	OE2	GLU	T	130	27.496	21.331	65.701	1.00	49.66	T	O
ATOM	4060	N	ARG	T	131	22.151	21.768	63.785	1.00	36.07	T	N
ATOM	4061	CA	ARG	T	131	21.590	22.024	62.473	1.00	34.72	T	C
ATOM	4062	C	ARG	T	131	22.631	21.836	61.377	1.00	32.32	T	C
ATOM	4063	O	ARG	T	131	23.838	21.925	61.612	1.00	30.97	T	O
ATOM	4064	CB	ARG	T	131	21.000	23.436	62.402	1.00	37.34	T	C
ATOM	4065	CG	ARG	T	131	21.948	24.547	62.807	1.00	41.83	T	C
ATOM	4066	CD	ARG	T	131	21.330	25.901	62.509	1.00	43.91	T	C
ATOM	4067	NE	ARG	T	131	22.022	26.999	63.178	1.00	45.56	T	N
ATOM	4068	CZ	ARG	T	131	21.691	28.280	63.048	1.00	45.22	T	C
ATOM	4069	NH1	ARG	T	131	20.679	28.634	62.265	1.00	44.75	T	N
ATOM	4070	NH2	ARG	T	131	22.362	29.208	63.715	1.00	46.22	T	N
ATOM	4071	N	THR	T	132	22.141	21.556	60.177	1.00	29.36	T	N
ATOM	4072	CA	THR	T	132	22.989	21.343	59.013	1.00	25.98	T	C
ATOM	4073	C	THR	T	132	22.664	22.438	58.008	1.00	26.04	T	C
ATOM	4074	O	THR	T	132	21.750	23.236	58.220	1.00	25.67	T	O
ATOM	4075	CB	THR	T	132	22.689	19.986	58.351	1.00	24.12	T	C
ATOM	4076	OG1	THR	T	132	21.425	20.061	57.680	1.00	19.80	T	O
ATOM	4077	CG2	THR	T	132	22.621	18.874	59.403	1.00	22.09	T	C
ATOM	4078	N	LEU	T	133	23.410	22.471	56.912	1.00	26.23	T	N
ATOM	4079	CA	LEU	T	133	23.181	23.459	55.867	1.00	28.66	T	C

ATOM	4080	C	LEU	T	133	22.060	23.029	54.922	1.00	31.07	T	C
ATOM	4081	O	LEU	T	133	21.664	23.788	54.038	1.00	31.66	T	O
ATOM	4082	CB	LEU	T	133	24.466	23.700	55.069	1.00	25.94	T	C
ATOM	4083	CG	LEU	T	133	25.457	24.719	55.645	1.00	24.82	T	C
ATOM	4084	CD1	LEU	T	133	24.818	26.095	55.618	1.00	23.33	T	C
ATOM	4085	CD2	LEU	T	133	25.873	24.336	57.068	1.00	23.50	T	C
ATOM	4086	N	VAL	T	134	21.553	21.812	55.104	1.00	32.72	T	N
ATOM	4087	CA	VAL	T	134	20.475	21.309	54.260	1.00	35.27	T	C
ATOM	4088	C	VAL	T	134	19.203	22.086	54.557	1.00	37.69	T	C
ATOM	4089	O	VAL	T	134	18.691	22.045	55.671	1.00	37.30	T	O
ATOM	4090	CB	VAL	T	134	20.207	19.803	54.508	1.00	33.94	T	C
ATOM	4091	CG1	VAL	T	134	19.038	19.335	53.652	1.00	31.92	T	C
ATOM	4092	CG2	VAL	T	134	21.453	18.992	54.189	1.00	30.88	T	C
ATOM	4093	N	ARG	T	135	18.702	22.803	53.558	1.00	42.86	T	N
ATOM	4094	CA	ARG	T	135	17.485	23.587	53.720	1.00	48.17	T	C
ATOM	4095	C	ARG	T	135	16.268	22.895	53.123	1.00	51.28	T	C
ATOM	4096	O	ARG	T	135	16.332	22.333	52.031	1.00	52.30	T	O
ATOM	4097	CB	ARG	T	135	17.636	24.960	53.063	1.00	48.77	T	C
ATOM	4098	CG	ARG	T	135	17.844	26.107	54.032	1.00	51.28	T	C
ATOM	4099	CD	ARG	T	135	17.150	27.366	53.522	1.00	53.42	T	C
ATOM	4100	NE	ARG	T	135	17.342	28.513	54.408	1.00	54.39	T	N
ATOM	4101	CZ	ARG	T	135	18.442	29.260	54.454	1.00	54.74	T	C
ATOM	4102	NH1	ARG	T	135	19.473	28.995	53.659	1.00	53.86	T	N
ATOM	4103	NH2	ARG	T	135	18.512	30.276	55.303	1.00	55.25	T	N
ATOM	4104	N	ARG	T	136	15.161	22.938	53.855	1.00	55.32	T	N
ATOM	4105	CA	ARG	T	136	13.905	22.355	53.401	1.00	59.86	T	C
ATOM	4106	C	ARG	T	136	12.764	23.218	53.912	1.00	60.84	T	C
ATOM	4107	O	ARG	T	136	12.685	23.514	55.105	1.00	60.73	T	O
ATOM	4108	CB	ARG	T	136	13.740	20.917	53.903	1.00	62.06	T	C
ATOM	4109	CG	ARG	T	136	14.704	19.926	53.266	1.00	65.96	T	C
ATOM	4110	CD	ARG	T	136	14.066	18.552	53.079	1.00	68.51	T	C
ATOM	4111	NE	ARG	T	136	13.514	18.011	54.320	1.00	71.12	T	N
ATOM	4112	CZ	ARG	T	136	13.019	16.784	54.453	1.00	72.57	T	C
ATOM	4113	NH1	ARG	T	136	12.999	15.951	53.420	1.00	73.26	T	N
ATOM	4114	NH2	ARG	T	136	12.542	16.387	55.625	1.00	73.03	T	N
ATOM	4115	N	ASN	T	137	11.888	23.623	52.998	1.00	62.35	T	N
ATOM	4116	CA	ASN	T	137	10.751	24.473	53.330	1.00	63.21	T	C
ATOM	4117	C	ASN	T	137	11.254	25.891	53.602	1.00	62.33	T	C
ATOM	4118	O	ASN	T	137	11.409	26.685	52.674	1.00	63.22	T	O
ATOM	4119	CB	ASN	T	137	10.001	23.924	54.552	1.00	65.32	T	C
ATOM	4120	CG	ASN	T	137	9.422	22.542	54.311	1.00	67.61	T	C
ATOM	4121	OD1	ASN	T	137	10.147	21.596	54.002	1.00	69.63	T	O
ATOM	4122	ND2	ASN	T	137	8.108	22.419	54.456	1.00	69.48	T	N
ATOM	4123	N	ASN	T	138	11.518	26.205	54.867	1.00	60.71	T	N
ATOM	4124	CA	ASN	T	138	12.003	27.531	55.234	1.00	58.80	T	C
ATOM	4125	C	ASN	T	138	12.940	27.486	56.445	1.00	56.17	T	C
ATOM	4126	O	ASN	T	138	13.061	28.467	57.179	1.00	56.57	T	O
ATOM	4127	CB	ASN	T	138	10.823	28.464	55.542	1.00	60.66	T	C
ATOM	4128	CG	ASN	T	138	9.842	28.582	54.381	1.00	62.38	T	C
ATOM	4129	OD1	ASN	T	138	9.132	27.631	54.049	1.00	62.68	T	O
ATOM	4130	ND2	ASN	T	138	9.801	29.756	53.760	1.00	63.11	T	N
ATOM	4131	N	THR	T	139	13.606	26.352	56.649	1.00	52.17	T	N
ATOM	4132	CA	THR	T	139	14.520	26.197	57.777	1.00	48.11	T	C
ATOM	4133	C	THR	T	139	15.641	25.203	57.483	1.00	43.77	T	C
ATOM	4134	O	THR	T	139	15.649	24.548	56.442	1.00	43.95	T	O
ATOM	4135	CB	THR	T	139	13.772	25.709	59.040	1.00	49.28	T	C

ATOM	4136	OG1	THR	T	139	13.085	24.486	58.745	1.00	48.22	T	O
ATOM	4137	CG2	THR	T	139	12.771	26.755	59.516	1.00	49.39	T	C
ATOM	4138	N	PHE	T	140	16.586	25.102	58.412	1.00	39.50	T	N
ATOM	4139	CA	PHE	T	140	17.713	24.184	58.284	1.00	34.81	T	C
ATOM	4140	C	PHE	T	140	17.369	22.876	58.987	1.00	33.69	T	C
ATOM	4141	O	PHE	T	140	16.857	22.884	60.107	1.00	33.95	T	O
ATOM	4142	CB	PHE	T	140	18.968	24.782	58.924	1.00	31.68	T	C
ATOM	4143	CG	PHE	T	140	19.538	25.956	58.177	1.00	29.78	T	C
ATOM	4144	CD1	PHE	T	140	20.222	25.772	56.980	1.00	28.87	T	C
ATOM	4145	CD2	PHE	T	140	19.404	27.247	58.679	1.00	29.29	T	C
ATOM	4146	CE1	PHE	T	140	20.770	26.856	56.293	1.00	27.26	T	C
ATOM	4147	CE2	PHE	T	140	19.948	28.341	57.999	1.00	28.58	T	C
ATOM	4148	CZ	PHE	T	140	20.634	28.142	56.803	1.00	26.93	T	C
ATOM	4149	N	LEU	T	141	17.648	21.758	58.325	1.00	31.02	T	N
ATOM	4150	CA	LEU	T	141	17.374	20.446	58.890	1.00	29.31	T	C
ATOM	4151	C	LEU	T	141	18.484	20.056	59.849	1.00	28.67	T	C
ATOM	4152	O	LEU	T	141	19.654	20.369	59.623	1.00	27.90	T	O
ATOM	4153	CB	LEU	T	141	17.285	19.389	57.788	1.00	28.83	T	C
ATOM	4154	CG	LEU	T	141	16.220	19.545	56.706	1.00	29.79	T	C
ATOM	4155	CD1	LEU	T	141	16.308	18.356	55.761	1.00	27.88	T	C
ATOM	4156	CD2	LEU	T	141	14.836	19.634	57.340	1.00	29.65	T	C
ATOM	4157	N	SER	T	142	18.116	19.359	60.916	1.00	26.59	T	N
ATOM	4158	CA	SER	T	142	19.095	18.930	61.900	1.00	25.72	T	C
ATOM	4159	C	SER	T	142	19.815	17.689	61.389	1.00	25.43	T	C
ATOM	4160	O	SER	T	142	19.422	17.099	60.380	1.00	24.69	T	O
ATOM	4161	CB	SER	T	142	18.405	18.617	63.225	1.00	24.53	T	C
ATOM	4162	OG	SER	T	142	17.693	17.393	63.142	1.00	27.31	T	O
ATOM	4163	N	LEU	T	143	20.866	17.287	62.095	1.00	25.42	T	N
ATOM	4164	CA	LEU	T	143	21.632	16.117	61.700	1.00	26.13	T	C
ATOM	4165	C	LEU	T	143	20.765	14.862	61.714	1.00	27.25	T	C
ATOM	4166	O	LEU	T	143	20.931	13.973	60.875	1.00	27.17	T	O
ATOM	4167	CB	LEU	T	143	22.830	15.936	62.630	1.00	28.10	T	C
ATOM	4168	CG	LEU	T	143	23.975	15.082	62.080	1.00	29.38	T	C
ATOM	4169	CD1	LEU	T	143	24.572	15.759	60.854	1.00	30.74	T	C
ATOM	4170	CD2	LEU	T	143	25.041	14.903	63.153	1.00	33.30	T	C
ATOM	4171	N	ARG	T	144	19.837	14.778	62.662	1.00	28.42	T	N
ATOM	4172	CA	ARG	T	144	18.973	13.609	62.721	1.00	29.34	T	C
ATOM	4173	C	ARG	T	144	17.850	13.700	61.687	1.00	29.34	T	C
ATOM	4174	O	ARG	T	144	17.338	12.676	61.244	1.00	30.63	T	O
ATOM	4175	CB	ARG	T	144	18.403	13.411	64.127	1.00	28.19	T	C
ATOM	4176	CG	ARG	T	144	17.727	12.059	64.285	1.00	29.87	T	C
ATOM	4177	CD	ARG	T	144	17.594	11.638	65.736	1.00	29.47	T	C
ATOM	4178	NE	ARG	T	144	18.861	11.246	66.358	1.00	29.59	T	N
ATOM	4179	CZ	ARG	T	144	19.587	10.183	66.017	1.00	28.70	T	C
ATOM	4180	NH1	ARG	T	144	19.195	9.378	65.039	1.00	28.08	T	N
ATOM	4181	NH2	ARG	T	144	20.699	9.904	66.682	1.00	27.54	T	N
ATOM	4182	N	ASP	T	145	17.469	14.918	61.301	1.00	29.51	T	N
ATOM	4183	CA	ASP	T	145	16.438	15.093	60.275	1.00	30.78	T	C
ATOM	4184	C	ASP	T	145	16.940	14.472	58.970	1.00	29.67	T	C
ATOM	4185	O	ASP	T	145	16.195	13.793	58.263	1.00	30.38	T	O
ATOM	4186	CB	ASP	T	145	16.147	16.578	60.007	1.00	31.56	T	C
ATOM	4187	CG	ASP	T	145	15.239	17.204	61.048	1.00	33.74	T	C
ATOM	4188	OD1	ASP	T	145	14.327	16.520	61.530	1.00	37.12	T	O
ATOM	4189	OD2	ASP	T	145	15.430	18.385	61.356	1.00	31.92	T	O
ATOM	4190	N	VAL	T	146	18.215	14.719	58.670	1.00	27.99	T	N
ATOM	4191	CA	VAL	T	146	18.871	14.231	57.459	1.00	25.95	T	C

ATOM	4192	C	VAL	T	146	19.245	12.750	57.474	1.00	26.46	T	C
ATOM	4193	O	VAL	T	146	18.922	12.024	56.541	1.00	27.73	T	O
ATOM	4194	CB	VAL	T	146	20.168	15.048	57.164	1.00	24.95	T	C
ATOM	4195	CG1	VAL	T	146	20.901	14.461	55.960	1.00	20.92	T	C
ATOM	4196	CG2	VAL	T	146	19.823	16.519	56.916	1.00	20.74	T	C
ATOM	4197	N	PHE	T	147	19.929	12.305	58.524	1.00	26.36	T	N
ATOM	4198	CA	PHE	T	147	20.369	10.912	58.619	1.00	25.98	T	C
ATOM	4199	C	PHE	T	147	19.379	9.919	59.236	1.00	27.12	T	C
ATOM	4200	O	PHE	T	147	19.536	8.708	59.084	1.00	25.23	T	O
ATOM	4201	CB	PHE	T	147	21.689	10.844	59.389	1.00	24.48	T	C
ATOM	4202	CG	PHE	T	147	22.844	11.465	58.662	1.00	25.86	T	C
ATOM	4203	CD1	PHE	T	147	23.388	10.848	57.546	1.00	25.81	T	C
ATOM	4204	CD2	PHE	T	147	23.377	12.681	59.082	1.00	26.68	T	C
ATOM	4205	CE1	PHE	T	147	24.450	11.429	56.852	1.00	27.09	T	C
ATOM	4206	CE2	PHE	T	147	24.435	13.267	58.398	1.00	26.05	T	C
ATOM	4207	CZ	PHE	T	147	24.972	12.639	57.280	1.00	25.43	T	C
ATOM	4208	N	GLY	T	148	18.368	10.421	59.930	1.00	27.07	T	N
ATOM	4209	CA	GLY	T	148	17.406	9.526	60.542	1.00	30.74	T	C
ATOM	4210	C	GLY	T	148	18.079	8.427	61.347	1.00	31.33	T	C
ATOM	4211	O	GLY	T	148	18.894	8.710	62.227	1.00	31.75	T	O
ATOM	4212	N	LYS	T	149	17.757	7.174	61.033	1.00	31.90	T	N
ATOM	4213	CA	LYS	T	149	18.319	6.024	61.745	1.00	30.48	T	C
ATOM	4214	C	LYS	T	149	19.784	5.707	61.448	1.00	29.20	T	C
ATOM	4215	O	LYS	T	149	20.391	4.894	62.143	1.00	28.53	T	O
ATOM	4216	CB	LYS	T	149	17.480	4.771	61.475	1.00	32.10	T	C
ATOM	4217	CG	LYS	T	149	17.526	4.284	60.036	1.00	34.68	T	C
ATOM	4218	CD	LYS	T	149	16.654	3.045	59.849	1.00	38.94	T	C
ATOM	4219	CE	LYS	T	149	16.596	2.617	58.390	1.00	39.85	T	C
ATOM	4220	NZ	LYS	T	149	17.943	2.260	57.865	1.00	42.88	T	N
ATOM	4221	N	ASP	T	150	20.356	6.318	60.416	1.00	28.28	T	N
ATOM	4222	CA	ASP	T	150	21.763	6.060	60.103	1.00	27.67	T	C
ATOM	4223	C	ASP	T	150	22.698	6.678	61.142	1.00	26.20	T	C
ATOM	4224	O	ASP	T	150	23.859	6.283	61.257	1.00	26.29	T	O
ATOM	4225	CB	ASP	T	150	22.137	6.620	58.727	1.00	28.41	T	C
ATOM	4226	CG	ASP	T	150	21.631	5.765	57.592	1.00	30.84	T	C
ATOM	4227	OD1	ASP	T	150	21.557	4.547	57.765	1.00	30.37	T	O
ATOM	4228	OD2	ASP	T	150	21.330	6.319	56.530	1.00	31.25	T	O
ATOM	4229	N	LEU	T	151	22.186	7.645	61.897	1.00	24.20	T	N
ATOM	4230	CA	LEU	T	151	22.978	8.342	62.901	1.00	24.32	T	C
ATOM	4231	C	LEU	T	151	22.800	7.847	64.333	1.00	23.19	T	C
ATOM	4232	O	LEU	T	151	21.681	7.654	64.805	1.00	23.35	T	O
ATOM	4233	CB	LEU	T	151	22.651	9.839	62.858	1.00	23.48	T	C
ATOM	4234	CG	LEU	T	151	23.299	10.741	63.916	1.00	24.55	T	C
ATOM	4235	CD1	LEU	T	151	24.791	10.863	63.649	1.00	21.55	T	C
ATOM	4236	CD2	LEU	T	151	22.638	12.117	63.885	1.00	24.04	T	C
ATOM	4237	N	ILE	T	152	23.917	7.639	65.020	1.00	23.69	T	N
ATOM	4238	CA	ILE	T	152	23.882	7.235	66.419	1.00	23.13	T	C
ATOM	4239	C	ILE	T	152	24.886	8.111	67.154	1.00	23.28	T	C
ATOM	4240	O	ILE	T	152	25.736	8.752	66.537	1.00	24.54	T	O
ATOM	4241	CB	ILE	T	152	24.287	5.747	66.643	1.00	22.81	T	C
ATOM	4242	CG1	ILE	T	152	25.799	5.584	66.493	1.00	22.58	T	C
ATOM	4243	CG2	ILE	T	152	23.534	4.839	65.672	1.00	23.41	T	C
ATOM	4244	CD1	ILE	T	152	26.322	4.228	66.945	1.00	22.76	T	C
ATOM	4245	N	TYR	T	153	24.779	8.150	68.472	1.00	23.49	T	N
ATOM	4246	CA	TYR	T	153	25.711	8.920	69.271	1.00	24.51	T	C
ATOM	4247	C	TYR	T	153	26.359	7.984	70.274	1.00	24.18	T	C

ATOM	4248	O	TYR	T	153	25.715	7.078	70.802	1.00	24.71	T	O
ATOM	4249	CB	TYR	T	153	24.995	10.067	69.984	1.00	23.68	T	C
ATOM	4250	CG	TYR	T	153	24.745	11.256	69.081	1.00	23.64	T	C
ATOM	4251	CD1	TYR	T	153	25.805	12.036	68.623	1.00	23.71	T	C
ATOM	4252	CD2	TYR	T	153	23.454	11.597	68.677	1.00	22.84	T	C
ATOM	4253	CE1	TYR	T	153	25.590	13.130	67.786	1.00	21.55	T	C
ATOM	4254	CE2	TYR	T	153	23.226	12.690	67.839	1.00	22.98	T	C
ATOM	4255	CZ	TYR	T	153	24.301	13.450	67.399	1.00	22.00	T	C
ATOM	4256	OH	TYR	T	153	24.092	14.527	66.575	1.00	21.50	T	O
ATOM	4257	N	THR	T	154	27.647	8.193	70.506	1.00	23.44	T	N
ATOM	4258	CA	THR	T	154	28.403	7.381	71.438	1.00	23.84	T	C
ATOM	4259	C	THR	T	154	28.830	8.250	72.615	1.00	25.48	T	C
ATOM	4260	O	THR	T	154	29.260	9.387	72.431	1.00	25.59	T	O
ATOM	4261	CB	THR	T	154	29.640	6.783	70.741	1.00	24.28	T	C
ATOM	4262	OG1	THR	T	154	29.212	5.846	69.742	1.00	24.66	T	O
ATOM	4263	CG2	THR	T	154	30.540	6.081	71.740	1.00	27.90	T	C
ATOM	4264	N	LEU	T	155	28.685	7.715	73.822	1.00	26.46	T	N
ATOM	4265	CA	LEU	T	155	29.056	8.428	75.036	1.00	29.00	T	C
ATOM	4266	C	LEU	T	155	30.286	7.788	75.670	1.00	31.35	T	C
ATOM	4267	O	LEU	T	155	30.356	6.570	75.831	1.00	33.70	T	O
ATOM	4268	CB	LEU	T	155	27.894	8.416	76.039	1.00	26.23	T	C
ATOM	4269	CG	LEU	T	155	28.112	9.127	77.381	1.00	26.86	T	C
ATOM	4270	CD1	LEU	T	155	28.263	10.620	77.155	1.00	25.42	T	C
ATOM	4271	CD2	LEU	T	155	26.941	8.851	78.307	1.00	24.97	T	C
ATOM	4272	N	TYR	T	156	31.254	8.625	76.014	1.00	33.72	T	N
ATOM	4273	CA	TYR	T	156	32.494	8.198	76.649	1.00	36.80	T	C
ATOM	4274	C	TYR	T	156	32.466	8.870	78.016	1.00	37.49	T	C
ATOM	4275	O	TYR	T	156	32.747	10.061	78.125	1.00	37.28	T	O
ATOM	4276	CB	TYR	T	156	33.690	8.703	75.835	1.00	39.78	T	C
ATOM	4277	CG	TYR	T	156	35.056	8.392	76.413	1.00	44.27	T	C
ATOM	4278	CD1	TYR	T	156	35.633	7.130	76.262	1.00	45.90	T	C
ATOM	4279	CD2	TYR	T	156	35.787	9.374	77.085	1.00	46.33	T	C
ATOM	4280	CE1	TYR	T	156	36.908	6.856	76.762	1.00	46.82	T	C
ATOM	4281	CE2	TYR	T	156	37.060	9.110	77.590	1.00	46.50	T	C
ATOM	4282	CZ	TYR	T	156	37.614	7.851	77.424	1.00	47.92	T	C
ATOM	4283	OH	TYR	T	156	38.875	7.593	77.914	1.00	48.85	T	O
ATOM	4284	N	TYR	T	157	32.098	8.113	79.047	1.00	38.10	T	N
ATOM	4285	CA	TYR	T	157	32.017	8.650	80.404	1.00	39.51	T	C
ATOM	4286	C	TYR	T	157	32.911	7.927	81.407	1.00	41.43	T	C
ATOM	4287	O	TYR	T	157	33.153	6.729	81.286	1.00	41.55	T	O
ATOM	4288	CB	TYR	T	157	30.566	8.627	80.905	1.00	37.07	T	C
ATOM	4289	CG	TYR	T	157	29.924	7.255	81.019	1.00	36.59	T	C
ATOM	4290	CD1	TYR	T	157	29.578	6.520	79.884	1.00	36.61	T	C
ATOM	4291	CD2	TYR	T	157	29.622	6.712	82.269	1.00	36.44	T	C
ATOM	4292	CE1	TYR	T	157	28.942	5.282	79.990	1.00	36.96	T	C
ATOM	4293	CE2	TYR	T	157	28.989	5.478	82.388	1.00	36.19	T	C
ATOM	4294	CZ	TYR	T	157	28.649	4.768	81.247	1.00	37.43	T	C
ATOM	4295	OH	TYR	T	157	28.011	3.554	81.362	1.00	35.29	T	O
ATOM	4296	N	TRP	T	158	33.393	8.666	82.402	1.00	44.59	T	N
ATOM	4297	CA	TRP	T	158	34.266	8.101	83.423	1.00	48.36	T	C
ATOM	4298	C	TRP	T	158	33.941	8.612	84.822	1.00	50.71	T	C
ATOM	4299	O	TRP	T	158	33.389	9.700	84.989	1.00	50.01	T	O
ATOM	4300	CB	TRP	T	158	35.727	8.414	83.092	1.00	48.77	T	C
ATOM	4301	CG	TRP	T	158	36.071	9.873	83.156	1.00	50.02	T	C
ATOM	4302	CD1	TRP	T	158	36.242	10.631	84.281	1.00	50.16	T	C
ATOM	4303	CD2	TRP	T	158	36.291	10.752	82.045	1.00	50.25	T	C

ATOM	4304	NE1	TRP	T	158	36.557	11.924	83.940	1.00	50.45	T	N
ATOM	4305	CE2	TRP	T	158	36.595	12.027	82.574	1.00	49.97	T	C
ATOM	4306	CE3	TRP	T	158	36.262	10.585	80.653	1.00	50.09	T	C
ATOM	4307	CZ2	TRP	T	158	36.869	13.131	81.760	1.00	49.43	T	C
ATOM	4308	CZ3	TRP	T	158	36.534	11.685	79.843	1.00	50.00	T	C
ATOM	4309	CH2	TRP	T	158	36.834	12.941	80.402	1.00	50.53	T	C
ATOM	4310	N	LYS	T	159	34.295	7.815	85.826	1.00	54.36	T	N
ATOM	4311	CA	LYS	T	159	34.053	8.167	87.220	1.00	57.78	T	C
ATOM	4312	C	LYS	T	159	35.218	9.024	87.735	1.00	58.65	T	C
ATOM	4313	O	LYS	T	159	35.371	10.173	87.325	1.00	60.01	T	O
ATOM	4314	CB	LYS	T	159	33.911	6.887	88.053	1.00	59.26	T	C
ATOM	4315	CG	LYS	T	159	33.266	7.081	89.416	1.00	61.42	T	C
ATOM	4316	CD	LYS	T	159	33.503	5.877	90.322	1.00	63.98	T	C
ATOM	4317	CE	LYS	T	159	32.979	4.584	89.712	1.00	65.42	T	C
ATOM	4318	NZ	LYS	T	159	31.501	4.599	89.542	1.00	67.11	T	N
ATOM	4319	N	SER	T	160	36.035	8.460	88.622	1.00	60.77	T	N
ATOM	4320	CA	SER	T	160	37.188	9.152	89.198	1.00	62.01	T	C
ATOM	4321	C	SER	T	160	37.933	8.228	90.157	1.00	62.68	T	C
ATOM	4322	O	SER	T	160	37.520	8.043	91.303	1.00	63.75	T	O
ATOM	4323	CB	SER	T	160	36.751	10.413	89.952	1.00	62.64	T	C
ATOM	4324	OG	SER	T	160	36.348	11.441	89.063	1.00	63.25	T	O
ATOM	4325	N	GLY	T	164	39.552	4.169	84.389	1.00	46.65	T	N
ATOM	4326	CA	GLY	T	164	38.188	3.681	84.302	1.00	46.62	T	C
ATOM	4327	C	GLY	T	164	37.414	4.314	83.161	1.00	45.68	T	C
ATOM	4328	O	GLY	T	164	36.884	5.415	83.296	1.00	45.48	T	O
ATOM	4329	N	LYS	T	165	37.347	3.611	82.036	1.00	45.62	T	N
ATOM	4330	CA	LYS	T	165	36.635	4.100	80.859	1.00	44.77	T	C
ATOM	4331	C	LYS	T	165	35.296	3.385	80.697	1.00	42.99	T	C
ATOM	4332	O	LYS	T	165	35.198	2.178	80.921	1.00	43.15	T	O
ATOM	4333	CB	LYS	T	165	37.480	3.885	79.593	1.00	47.71	T	C
ATOM	4334	CG	LYS	T	165	38.658	4.851	79.404	1.00	51.07	T	C
ATOM	4335	CD	LYS	T	165	39.777	4.652	80.424	1.00	53.07	T	C
ATOM	4336	CE	LYS	T	165	40.370	3.252	80.348	1.00	55.53	T	C
ATOM	4337	NZ	LYS	T	165	40.940	2.954	79.005	1.00	58.19	T	N
ATOM	4338	N	LYS	T	166	34.269	4.135	80.309	1.00	40.32	T	N
ATOM	4339	CA	LYS	T	166	32.937	3.573	80.103	1.00	38.29	T	C
ATOM	4340	C	LYS	T	166	32.325	4.137	78.818	1.00	36.09	T	C
ATOM	4341	O	LYS	T	166	32.609	5.268	78.427	1.00	32.41	T	O
ATOM	4342	CB	LYS	T	166	32.032	3.892	81.297	1.00	40.50	T	C
ATOM	4343	CG	LYS	T	166	32.510	3.306	82.617	1.00	43.96	T	C
ATOM	4344	CD	LYS	T	166	31.622	3.752	83.767	1.00	45.60	T	C
ATOM	4345	CE	LYS	T	166	32.151	3.265	85.107	1.00	47.87	T	C
ATOM	4346	NZ	LYS	T	166	31.334	3.791	86.239	1.00	49.02	T	N
ATOM	4347	N	THR	T	167	31.475	3.347	78.172	1.00	33.24	T	N
ATOM	4348	CA	THR	T	167	30.851	3.771	76.926	1.00	32.13	T	C
ATOM	4349	C	THR	T	167	29.386	3.355	76.799	1.00	30.44	T	C
ATOM	4350	O	THR	T	167	28.969	2.318	77.316	1.00	29.24	T	O
ATOM	4351	CB	THR	T	167	31.623	3.205	75.719	1.00	33.05	T	C
ATOM	4352	OG1	THR	T	167	31.000	3.632	74.502	1.00	34.90	T	O
ATOM	4353	CG2	THR	T	167	31.633	1.686	75.767	1.00	34.83	T	C
ATOM	4354	N	ALA	T	168	28.616	4.184	76.102	1.00	27.66	T	N
ATOM	4355	CA	ALA	T	168	27.201	3.934	75.866	1.00	27.24	T	C
ATOM	4356	C	ALA	T	168	26.887	4.359	74.434	1.00	26.54	T	C
ATOM	4357	O	ALA	T	168	27.614	5.159	73.853	1.00	26.79	T	O
ATOM	4358	CB	ALA	T	168	26.356	4.738	76.847	1.00	25.11	T	C
ATOM	4359	N	LYS	T	169	25.815	3.818	73.864	1.00	25.71	T	N

ATOM	4360	CA	LYS	T	169	25.421	4.174	72.503	1.00	24.30	T	C
ATOM	4361	C	LYS	T	169	23.912	4.341	72.416	1.00	23.34	T	C
ATOM	4362	O	LYS	T	169	23.165	3.613	73.056	1.00	25.30	T	O
ATOM	4363	CB	LYS	T	169	25.898	3.108	71.519	1.00	25.23	T	C
ATOM	4364	CG	LYS	T	169	27.401	2.925	71.531	1.00	24.44	T	C
ATOM	4365	CD	LYS	T	169	27.864	1.937	70.489	1.00	25.08	T	C
ATOM	4366	CE	LYS	T	169	29.368	1.780	70.552	1.00	22.30	T	C
ATOM	4367	NZ	LYS	T	169	29.879	1.009	69.398	1.00	25.32	T	N
ATOM	4368	N	THR	T	170	23.467	5.309	71.625	1.00	24.63	T	N
ATOM	4369	CA	THR	T	170	22.040	5.574	71.475	1.00	24.26	T	C
ATOM	4370	C	THR	T	170	21.680	5.871	70.023	1.00	26.19	T	C
ATOM	4371	O	THR	T	170	22.491	6.408	69.269	1.00	26.16	T	O
ATOM	4372	CB	THR	T	170	21.607	6.783	72.335	1.00	22.44	T	C
ATOM	4373	OG1	THR	T	170	20.202	7.008	72.178	1.00	21.98	T	O
ATOM	4374	CG2	THR	T	170	22.361	8.040	71.907	1.00	20.38	T	C
ATOM	4375	N	ASN	T	171	20.463	5.518	69.631	1.00	27.31	T	N
ATOM	4376	CA	ASN	T	171	20.018	5.777	68.272	1.00	29.89	T	C
ATOM	4377	C	ASN	T	171	19.207	7.071	68.202	1.00	28.86	T	C
ATOM	4378	O	ASN	T	171	18.659	7.416	67.158	1.00	30.77	T	O
ATOM	4379	CB	ASN	T	171	19.201	4.596	67.744	1.00	34.19	T	C
ATOM	4380	CG	ASN	T	171	17.917	4.401	68.497	1.00	38.11	T	C
ATOM	4381	OD1	ASN	T	171	17.919	4.219	69.714	1.00	43.07	T	O
ATOM	4382	ND2	ASN	T	171	16.803	4.433	67.778	1.00	42.28	T	N
ATOM	4383	N	THR	T	172	19.129	7.781	69.324	1.00	27.79	T	N
ATOM	4384	CA	THR	T	172	18.432	9.063	69.385	1.00	27.05	T	C
ATOM	4385	C	THR	T	172	19.487	10.072	69.863	1.00	26.35	T	C
ATOM	4386	O	THR	T	172	20.678	9.898	69.593	1.00	24.98	T	O
ATOM	4387	CB	THR	T	172	17.242	9.030	70.381	1.00	26.35	T	C
ATOM	4388	OG1	THR	T	172	17.732	8.790	71.704	1.00	29.03	T	O
ATOM	4389	CG2	THR	T	172	16.258	7.930	70.009	1.00	26.97	T	C
ATOM	4390	N	ASN	T	173	19.065	11.119	70.559	1.00	24.76	T	N
ATOM	4391	CA	ASN	T	173	20.008	12.112	71.061	1.00	26.67	T	C
ATOM	4392	C	ASN	T	173	20.147	12.074	72.578	1.00	26.96	T	C
ATOM	4393	O	ASN	T	173	20.741	12.974	73.167	1.00	26.63	T	O
ATOM	4394	CB	ASN	T	173	19.583	13.517	70.632	1.00	27.09	T	C
ATOM	4395	CG	ASN	T	173	19.974	13.829	69.206	1.00	27.88	T	C
ATOM	4396	OD1	ASN	T	173	19.682	13.064	68.291	1.00	28.96	T	O
ATOM	4397	ND2	ASN	T	173	20.642	14.960	69.009	1.00	29.78	T	N
ATOM	4398	N	GLU	T	174	19.617	11.028	73.206	1.00	26.96	T	N
ATOM	4399	CA	GLU	T	174	19.680	10.906	74.659	1.00	28.12	T	C
ATOM	4400	C	GLU	T	174	20.340	9.619	75.143	1.00	26.22	T	C
ATOM	4401	O	GLU	T	174	20.215	8.569	74.523	1.00	26.38	T	O
ATOM	4402	CB	GLU	T	174	18.268	11.012	75.241	1.00	32.01	T	C
ATOM	4403	CG	GLU	T	174	17.604	12.365	74.996	1.00	39.60	T	C
ATOM	4404	CD	GLU	T	174	16.095	12.313	75.150	1.00	45.20	T	C
ATOM	4405	OE1	GLU	T	174	15.439	11.627	74.350	1.00	47.98	T	O
ATOM	4406	OE2	GLU	T	174	15.575	12.951	76.068	1.00	49.78	T	O
ATOM	4407	N	PHE	T	175	21.047	9.722	76.262	1.00	26.73	T	N
ATOM	4408	CA	PHE	T	175	21.730	8.591	76.877	1.00	26.52	T	C
ATOM	4409	C	PHE	T	175	21.161	8.402	78.280	1.00	29.29	T	C
ATOM	4410	O	PHE	T	175	21.052	9.367	79.037	1.00	29.51	T	O
ATOM	4411	CB	PHE	T	175	23.228	8.873	77.012	1.00	23.85	T	C
ATOM	4412	CG	PHE	T	175	23.968	8.919	75.710	1.00	23.33	T	C
ATOM	4413	CD1	PHE	T	175	24.315	7.743	75.051	1.00	22.59	T	C
ATOM	4414	CD2	PHE	T	175	24.345	10.139	75.154	1.00	21.95	T	C
ATOM	4415	CE1	PHE	T	175	25.034	7.780	73.851	1.00	24.26	T	C

ATOM	4416	CE2	PHE	T	175	25.063	10.189	73.956	1.00	23.03	T C
ATOM	4417	CZ	PHE	T	175	25.408	9.006	73.304	1.00	22.27	T C
ATOM	4418	N	LEU	T	176	20.791	7.171	78.622	1.00	31.93	T N
ATOM	4419	CA	LEU	T	176	20.276	6.873	79.959	1.00	34.35	T C
ATOM	4420	C	LEU	T	176	21.250	5.879	80.574	1.00	35.33	T C
ATOM	4421	O	LEU	T	176	21.255	4.705	80.211	1.00	36.35	T O
ATOM	4422	CB	LEU	T	176	18.876	6.254	79.890	1.00	34.93	T C
ATOM	4423	CG	LEU	T	176	18.220	5.937	81.243	1.00	36.34	T C
ATOM	4424	CD1	LEU	T	176	18.026	7.218	82.039	1.00	36.74	T C
ATOM	4425	CD2	LEU	T	176	16.876	5.250	81.022	1.00	37.90	T C
ATOM	4426	N	ILE	T	177	22.083	6.355	81.494	1.00	36.14	T N
ATOM	4427	CA	ILE	T	177	23.080	5.500	82.125	1.00	38.18	T C
ATOM	4428	C	ILE	T	177	22.968	5.430	83.643	1.00	39.89	T C
ATOM	4429	O	ILE	T	177	22.350	6.284	84.274	1.00	38.85	T O
ATOM	4430	CB	ILE	T	177	24.510	5.974	81.795	1.00	38.42	T C
ATOM	4431	CG1	ILE	T	177	24.750	7.358	82.407	1.00	38.45	T C
ATOM	4432	CG2	ILE	T	177	24.712	6.009	80.288	1.00	38.52	T C
ATOM	4433	CD1	ILE	T	177	26.208	7.791	82.420	1.00	39.58	T C
ATOM	4434	N	ASP	T	178	23.589	4.403	84.215	1.00	42.03	T N
ATOM	4435	CA	ASP	T	178	23.602	4.192	85.657	1.00	45.50	T C
ATOM	4436	C	ASP	T	178	24.802	4.914	86.259	1.00	47.95	T C
ATOM	4437	O	ASP	T	178	25.866	4.984	85.645	1.00	48.69	T O
ATOM	4438	CB	ASP	T	178	23.704	2.699	85.969	1.00	45.09	T C
ATOM	4439	CG	ASP	T	178	22.462	1.935	85.572	1.00	45.52	T C
ATOM	4440	OD1	ASP	T	178	22.561	0.737	85.367	1.00	46.53	T O
ATOM	4441	OD2	ASP	T	178	21.402	2.543	85.480	1.00	47.77	T O
ATOM	4442	N	VAL	T	179	24.630	5.447	87.463	1.00	51.00	T N
ATOM	4443	CA	VAL	T	179	25.709	6.158	88.138	1.00	54.37	T C
ATOM	4444	C	VAL	T	179	25.697	5.894	89.638	1.00	57.41	T C
ATOM	4445	O	VAL	T	179	24.634	5.808	90.257	1.00	58.33	T O
ATOM	4446	CB	VAL	T	179	25.610	7.684	87.912	1.00	53.68	T C
ATOM	4447	CG1	VAL	T	179	25.755	8.002	86.434	1.00	54.55	T C
ATOM	4448	CG2	VAL	T	179	24.285	8.206	88.445	1.00	53.15	T C
ATOM	4449	N	ASP	T	180	26.884	5.760	90.218	1.00	60.20	T N
ATOM	4450	CA	ASP	T	180	27.008	5.526	91.649	1.00	63.22	T C
ATOM	4451	C	ASP	T	180	26.787	6.854	92.363	1.00	64.55	T C
ATOM	4452	O	ASP	T	180	27.554	7.800	92.178	1.00	64.55	T O
ATOM	4453	CB	ASP	T	180	28.398	4.974	91.981	1.00	65.14	T C
ATOM	4454	CG	ASP	T	180	28.659	3.620	91.339	1.00	67.56	T C
ATOM	4455	OD1	ASP	T	180	28.706	3.545	90.113	1.00	69.02	T O
ATOM	4456	OD2	ASP	T	180	28.812	2.641	92.072	1.00	69.35	T O
ATOM	4457	N	LYS	T	181	25.730	6.924	93.169	1.00	66.14	T N
ATOM	4458	CA	LYS	T	181	25.400	8.145	93.900	1.00	66.70	T C
ATOM	4459	C	LYS	T	181	26.589	8.693	94.679	1.00	66.19	T C
ATOM	4460	O	LYS	T	181	27.464	7.941	95.110	1.00	66.44	T O
ATOM	4461	CB	LYS	T	181	24.230	7.895	94.858	1.00	68.20	T C
ATOM	4462	CG	LYS	T	181	22.910	7.573	94.166	1.00	70.66	T C
ATOM	4463	CD	LYS	T	181	21.747	7.534	95.154	1.00	71.98	T C
ATOM	4464	CE	LYS	T	181	21.915	6.434	96.194	1.00	73.05	T C
ATOM	4465	NZ	LYS	T	181	21.906	5.071	95.589	1.00	74.30	T N
ATOM	4466	N	GLY	T	182	26.613	10.011	94.851	1.00	65.88	T N
ATOM	4467	CA	GLY	T	182	27.698	10.647	95.578	1.00	65.07	T C
ATOM	4468	C	GLY	T	182	29.030	10.580	94.856	1.00	64.52	T C
ATOM	4469	O	GLY	T	182	30.085	10.552	95.488	1.00	64.76	T O
ATOM	4470	N	GLU	T	183	28.985	10.558	93.528	1.00	63.96	T N
ATOM	4471	CA	GLU	T	183	30.197	10.496	92.722	1.00	63.00	T C

ATOM	4472	C	GLU	T	183	30.012	11.349	91.471	1.00	60.60	T	C
ATOM	4473	O	GLU	T	183	28.948	11.336	90.854	1.00	60.74	T	O
ATOM	4474	CB	GLU	T	183	30.493	9.047	92.333	1.00	65.51	T	C
ATOM	4475	CG	GLU	T	183	31.877	8.829	91.749	1.00	69.10	T	C
ATOM	4476	CD	GLU	T	183	32.986	9.080	92.755	1.00	70.99	T	C
ATOM	4477	OE1	GLU	T	183	33.103	10.209	93.234	1.00	72.19	T	O
ATOM	4478	OE2	GLU	T	183	33.730	8.143	93.056	1.00	71.72	T	O
ATOM	4479	N	ASN	T	184	31.052	12.089	91.100	1.00	57.69	T	N
ATOM	4480	CA	ASN	T	184	30.987	12.959	89.933	1.00	54.65	T	C
ATOM	4481	C	ASN	T	184	31.475	12.282	88.654	1.00	51.10	T	C
ATOM	4482	O	ASN	T	184	32.494	11.589	88.647	1.00	49.50	T	O
ATOM	4483	CB	ASN	T	184	31.797	14.236	90.185	1.00	57.28	T	C
ATOM	4484	CG	ASN	T	184	31.324	14.996	91.415	1.00	59.82	T	C
ATOM	4485	OD1	ASN	T	184	31.448	14.517	92.545	1.00	62.30	T	O
ATOM	4486	ND2	ASN	T	184	30.775	16.187	91.200	1.00	60.42	T	N
ATOM	4487	N	TYR	T	185	30.733	12.492	87.572	1.00	46.87	T	N
ATOM	4488	CA	TYR	T	185	31.072	11.919	86.276	1.00	43.13	T	C
ATOM	4489	C	TYR	T	185	31.282	13.009	85.232	1.00	40.25	T	C
ATOM	4490	O	TYR	T	185	30.614	14.042	85.257	1.00	38.63	T	O
ATOM	4491	CB	TYR	T	185	29.955	10.999	85.772	1.00	42.93	T	C
ATOM	4492	CG	TYR	T	185	29.806	9.679	86.491	1.00	43.09	T	C
ATOM	4493	CD1	TYR	T	185	29.313	9.618	87.794	1.00	43.56	T	C
ATOM	4494	CD2	TYR	T	185	30.126	8.483	85.852	1.00	42.77	T	C
ATOM	4495	CE1	TYR	T	185	29.137	8.400	88.441	1.00	44.38	T	C
ATOM	4496	CE2	TYR	T	185	29.955	7.260	86.489	1.00	44.41	T	C
ATOM	4497	CZ	TYR	T	185	29.459	7.225	87.784	1.00	44.61	T	C
ATOM	4498	OH	TYR	T	185	29.273	6.016	88.413	1.00	46.20	T	O
ATOM	4499	N	CYS	T	186	32.215	12.773	84.318	1.00	37.22	T	N
ATOM	4500	CA	CYS	T	186	32.469	13.711	83.233	1.00	35.28	T	C
ATOM	4501	C	CYS	T	186	32.033	12.986	81.964	1.00	33.69	T	C
ATOM	4502	O	CYS	T	186	32.113	11.757	81.884	1.00	33.01	T	O
ATOM	4503	CB	CYS	T	186	33.948	14.084	83.145	1.00	34.62	T	C
ATOM	4504	SG	CYS	T	186	34.609	15.088	84.517	1.00	35.26	T	S
ATOM	4505	N	PHE	T	187	31.579	13.745	80.974	1.00	31.82	T	N
ATOM	4506	CA	PHE	T	187	31.085	13.164	79.737	1.00	29.80	T	C
ATOM	4507	C	PHE	T	187	31.657	13.778	78.465	1.00	28.26	T	C
ATOM	4508	O	PHE	T	187	32.121	14.918	78.451	1.00	25.87	T	O
ATOM	4509	CB	PHE	T	187	29.559	13.280	79.711	1.00	31.70	T	C
ATOM	4510	CG	PHE	T	187	28.892	12.750	80.950	1.00	32.92	T	C
ATOM	4511	CD1	PHE	T	187	28.783	11.381	81.167	1.00	32.88	T	C
ATOM	4512	CD2	PHE	T	187	28.401	13.623	81.919	1.00	34.37	T	C
ATOM	4513	CE1	PHE	T	187	28.196	10.887	82.330	1.00	32.44	T	C
ATOM	4514	CE2	PHE	T	187	27.812	13.137	83.088	1.00	33.58	T	C
ATOM	4515	CZ	PHE	T	187	27.711	11.767	83.292	1.00	33.15	T	C
ATOM	4516	N	SER	T	188	31.612	12.992	77.397	1.00	27.99	T	N
ATOM	4517	CA	SER	T	188	32.079	13.406	76.083	1.00	26.65	T	C
ATOM	4518	C	SER	T	188	31.324	12.557	75.071	1.00	26.06	T	C
ATOM	4519	O	SER	T	188	31.268	11.335	75.203	1.00	25.10	T	O
ATOM	4520	CB	SER	T	188	33.580	13.165	75.941	1.00	27.85	T	C
ATOM	4521	OG	SER	T	188	34.034	13.597	74.670	1.00	28.63	T	O
ATOM	4522	N	VAL	T	189	30.737	13.200	74.068	1.00	25.94	T	N
ATOM	4523	CA	VAL	T	189	29.977	12.476	73.056	1.00	25.53	T	C
ATOM	4524	C	VAL	T	189	30.585	12.579	71.667	1.00	26.44	T	C
ATOM	4525	O	VAL	T	189	31.397	13.462	71.381	1.00	27.25	T	O
ATOM	4526	CB	VAL	T	189	28.510	12.967	72.986	1.00	26.62	T	C
ATOM	4527	CG1	VAL	T	189	27.850	12.822	74.353	1.00	23.61	T	C

ATOM	4528	CG2	VAL	T	189	28.459	14.412	72.503	1.00	25.43	T	C
ATOM	4529	N	GLN	T	190	30.160	11.677	70.794	1.00	26.03	T	N
ATOM	4530	CA	GLN	T	190	30.670	11.627	69.438	1.00	25.75	T	C
ATOM	4531	C	GLN	T	190	29.562	11.173	68.495	1.00	24.90	T	C
ATOM	4532	O	GLN	T	190	28.825	10.238	68.803	1.00	24.21	T	O
ATOM	4533	CB	GLN	T	190	31.845	10.651	69.415	1.00	27.57	T	C
ATOM	4534	CG	GLN	T	190	32.563	10.466	68.103	1.00	29.40	T	C
ATOM	4535	CD	GLN	T	190	33.803	9.605	68.276	1.00	31.44	T	C
ATOM	4536	OE1	GLN	T	190	33.738	8.525	68.864	1.00	32.92	T	O
ATOM	4537	NE2	GLN	T	190	34.937	10.079	67.770	1.00	29.76	T	N
ATOM	4538	N	ALA	T	191	29.428	11.854	67.361	1.00	23.85	T	N
ATOM	4539	CA	ALA	T	191	28.415	11.496	66.374	1.00	22.47	T	C
ATOM	4540	C	ALA	T	191	29.016	10.401	65.504	1.00	22.81	T	C
ATOM	4541	O	ALA	T	191	30.212	10.424	65.214	1.00	22.19	T	O
ATOM	4542	CB	ALA	T	191	28.051	12.702	65.529	1.00	20.37	T	C
ATOM	4543	N	VAL	T	192	28.195	9.438	65.099	1.00	22.78	T	N
ATOM	4544	CA	VAL	T	192	28.684	8.332	64.286	1.00	23.06	T	C
ATOM	4545	C	VAL	T	192	27.636	7.854	63.285	1.00	25.12	T	C
ATOM	4546	O	VAL	T	192	26.435	7.911	63.549	1.00	25.90	T	O
ATOM	4547	CB	VAL	T	192	29.080	7.124	65.182	1.00	24.31	T	C
ATOM	4548	CG1	VAL	T	192	29.694	6.023	64.347	1.00	23.66	T	C
ATOM	4549	CG2	VAL	T	192	30.051	7.564	66.272	1.00	23.45	T	C
ATOM	4550	N	ILE	T	193	28.102	7.409	62.125	1.00	25.32	T	N
ATOM	4551	CA	ILE	T	193	27.233	6.856	61.098	1.00	27.61	T	C
ATOM	4552	C	ILE	T	193	27.881	5.519	60.772	1.00	29.11	T	C
ATOM	4553	O	ILE	T	193	28.734	5.429	59.887	1.00	31.58	T	O
ATOM	4554	CB	ILE	T	193	27.188	7.746	59.845	1.00	28.18	T	C
ATOM	4555	CG1	ILE	T	193	26.516	9.078	60.190	1.00	27.35	T	C
ATOM	4556	CG2	ILE	T	193	26.420	7.039	58.734	1.00	26.33	T	C
ATOM	4557	CD1	ILE	T	193	26.511	10.072	59.058	1.00	31.00	T	C
ATOM	4558	N	PRO	T	194	27.496	4.462	61.506	1.00	29.13	T	N
ATOM	4559	CA	PRO	T	194	28.006	3.091	61.360	1.00	30.19	T	C
ATOM	4560	C	PRO	T	194	28.153	2.557	59.940	1.00	29.68	T	C
ATOM	4561	O	PRO	T	194	29.168	1.954	59.605	1.00	30.22	T	O
ATOM	4562	CB	PRO	T	194	27.020	2.268	62.187	1.00	29.86	T	C
ATOM	4563	CG	PRO	T	194	26.631	3.224	63.273	1.00	30.63	T	C
ATOM	4564	CD	PRO	T	194	26.402	4.501	62.493	1.00	28.23	T	C
ATOM	4565	N	SER	T	195	27.142	2.773	59.109	1.00	31.11	T	N
ATOM	4566	CA	SER	T	195	27.172	2.294	57.732	1.00	33.61	T	C
ATOM	4567	C	SER	T	195	28.304	2.882	56.894	1.00	36.37	T	C
ATOM	4568	O	SER	T	195	28.653	2.331	55.848	1.00	37.68	T	O
ATOM	4569	CB	SER	T	195	25.841	2.594	57.049	1.00	33.34	T	C
ATOM	4570	OG	SER	T	195	25.592	3.987	57.025	1.00	33.89	T	O
ATOM	4571	N	ARG	T	196	28.876	3.994	57.350	1.00	37.43	T	N
ATOM	4572	CA	ARG	T	196	29.956	4.654	56.626	1.00	38.17	T	C
ATOM	4573	C	ARG	T	196	31.279	3.915	56.617	1.00	40.14	T	C
ATOM	4574	O	ARG	T	196	31.567	3.104	57.497	1.00	39.73	T	O
ATOM	4575	CB	ARG	T	196	30.201	6.055	57.181	1.00	36.13	T	C
ATOM	4576	CG	ARG	T	196	29.241	7.107	56.686	1.00	34.25	T	C
ATOM	4577	CD	ARG	T	196	29.764	8.479	57.042	1.00	33.30	T	C
ATOM	4578	NE	ARG	T	196	28.936	9.540	56.486	1.00	32.53	T	N
ATOM	4579	CZ	ARG	T	196	29.210	10.835	56.592	1.00	33.06	T	C
ATOM	4580	NH1	ARG	T	196	30.299	11.234	57.238	1.00	30.86	T	N
ATOM	4581	NH2	ARG	T	196	28.397	11.730	56.048	1.00	29.51	T	N
ATOM	4582	N	THR	T	197	32.082	4.227	55.604	1.00	42.50	T	N
ATOM	4583	CA	THR	T	197	33.405	3.645	55.435	1.00	43.94	T	C

ATOM	4584	C	THR	T	197	34.437	4.714	55.802	1.00	43.45	T C
ATOM	4585	O	THR	T	197	35.368	4.458	56.567	1.00	43.73	T O
ATOM	4586	CB	THR	T	197	33.623	3.181	53.976	1.00	45.61	T C
ATOM	4587	OG1	THR	T	197	33.452	4.291	53.086	1.00	48.03	T O
ATOM	4588	CG2	THR	T	197	32.618	2.094	53.608	1.00	46.03	T C
ATOM	4589	N	VAL	T	198	34.254	5.917	55.263	1.00	42.98	T N
ATOM	4590	CA	VAL	T	198	35.149	7.039	55.546	1.00	41.57	T C
ATOM	4591	C	VAL	T	198	34.383	8.062	56.371	1.00	38.54	T C
ATOM	4592	O	VAL	T	198	33.159	8.109	56.308	1.00	38.93	T O
ATOM	4593	CB	VAL	T	198	35.641	7.720	54.250	1.00	42.24	T C
ATOM	4594	CG1	VAL	T	198	36.388	6.713	53.390	1.00	43.81	T C
ATOM	4595	CG2	VAL	T	198	34.461	8.318	53.490	1.00	41.73	T C
ATOM	4596	N	ASN	T	199	35.104	8.882	57.133	1.00	36.53	T N
ATOM	4597	CA	ASN	T	199	34.483	9.898	57.985	1.00	34.68	T C
ATOM	4598	C	ASN	T	199	33.289	9.315	58.741	1.00	32.52	T C
ATOM	4599	O	ASN	T	199	32.201	9.884	58.732	1.00	31.11	T O
ATOM	4600	CB	ASN	T	199	34.016	11.092	57.147	1.00	36.34	T C
ATOM	4601	CG	ASN	T	199	35.137	11.723	56.352	1.00	38.20	T C
ATOM	4602	OD1	ASN	T	199	36.227	11.962	56.872	1.00	39.82	T O
ATOM	4603	ND2	ASN	T	199	34.871	12.012	55.083	1.00	38.88	T N
ATOM	4604	N	ARG	T	200	33.497	8.183	59.404	1.00	32.29	T N
ATOM	4605	CA	ARG	T	200	32.422	7.528	60.137	1.00	32.10	T C
ATOM	4606	C	ARG	T	200	32.098	8.205	61.459	1.00	29.78	T C
ATOM	4607	O	ARG	T	200	30.988	8.077	61.968	1.00	29.26	T O
ATOM	4608	CB	ARG	T	200	32.769	6.053	60.390	1.00	34.20	T C
ATOM	4609	CG	ARG	T	200	33.974	5.832	61.294	1.00	40.10	T C
ATOM	4610	CD	ARG	T	200	34.403	4.361	61.385	1.00	44.11	T C
ATOM	4611	NE	ARG	T	200	33.484	3.524	62.159	1.00	46.39	T N
ATOM	4612	CZ	ARG	T	200	32.419	2.896	61.665	1.00	46.92	T C
ATOM	4613	NH1	ARG	T	200	32.113	2.992	60.378	1.00	46.68	T N
ATOM	4614	NH2	ARG	T	200	31.656	2.161	62.465	1.00	47.08	T N
ATOM	4615	N	LYS	T	201	33.053	8.942	62.008	1.00	28.96	T N
ATOM	4616	CA	LYS	T	201	32.831	9.589	63.292	1.00	28.86	T C
ATOM	4617	C	LYS	T	201	33.277	11.042	63.325	1.00	26.57	T C
ATOM	4618	O	LYS	T	201	34.194	11.441	62.611	1.00	26.41	T O
ATOM	4619	CB	LYS	T	201	33.576	8.814	64.384	1.00	30.67	T C
ATOM	4620	CG	LYS	T	201	33.328	7.319	64.358	1.00	33.65	T C
ATOM	4621	CD	LYS	T	201	34.438	6.565	65.065	1.00	38.71	T C
ATOM	4622	CE	LYS	T	201	34.446	6.850	66.550	1.00	42.37	T C
ATOM	4623	NZ	LYS	T	201	33.187	6.371	67.184	1.00	45.63	T N
ATOM	4624	N	SER	T	202	32.614	11.830	64.161	1.00	25.68	T N
ATOM	4625	CA	SER	T	202	32.967	13.233	64.326	1.00	26.09	T C
ATOM	4626	C	SER	T	202	34.038	13.257	65.415	1.00	25.74	T C
ATOM	4627	O	SER	T	202	34.424	12.212	65.929	1.00	25.97	T O
ATOM	4628	CB	SER	T	202	31.754	14.033	64.803	1.00	25.44	T C
ATOM	4629	OG	SER	T	202	31.439	13.699	66.145	1.00	24.76	T O
ATOM	4630	N	THR	T	203	34.523	14.441	65.764	1.00	25.64	T N
ATOM	4631	CA	THR	T	203	35.507	14.545	66.829	1.00	26.70	T C
ATOM	4632	C	THR	T	203	34.734	14.575	68.150	1.00	26.56	T C
ATOM	4633	O	THR	T	203	33.542	14.890	68.170	1.00	26.32	T O
ATOM	4634	CB	THR	T	203	36.333	15.839	66.709	1.00	27.27	T C
ATOM	4635	OG1	THR	T	203	35.447	16.964	66.678	1.00	29.25	T O
ATOM	4636	CG2	THR	T	203	37.178	15.821	65.441	1.00	26.74	T C
ATOM	4637	N	ASP	T	204	35.407	14.244	69.247	1.00	26.24	T N
ATOM	4638	CA	ASP	T	204	34.775	14.245	70.561	1.00	25.07	T C
ATOM	4639	C	ASP	T	204	34.287	15.648	70.904	1.00	23.20	T C

ATOM	4640	O	ASP	T	204	34.926	16.638	70.557	1.00	22.85	T	O
ATOM	4641	CB	ASP	T	204	35.774	13.781	71.629	1.00	26.47	T	C
ATOM	4642	CG	ASP	T	204	36.322	12.384	71.360	1.00	28.96	T	C
ATOM	4643	OD1	ASP	T	204	35.559	11.414	71.438	1.00	28.17	T	O
ATOM	4644	OD2	ASP	T	204	37.515	12.269	71.071	1.00	31.64	T	O
ATOM	4645	N	SER	T	205	33.147	15.728	71.580	1.00	22.21	T	N
ATOM	4646	CA	SER	T	205	32.580	17.009	71.994	1.00	21.13	T	C
ATOM	4647	C	SER	T	205	33.383	17.532	73.179	1.00	20.53	T	C
ATOM	4648	O	SER	T	205	34.233	16.828	73.720	1.00	21.01	T	O
ATOM	4649	CB	SER	T	205	31.136	16.818	72.458	1.00	24.15	T	C
ATOM	4650	OG	SER	T	205	31.104	16.109	73.694	1.00	22.18	T	O
ATOM	4651	N	PRO	T	206	33.141	18.786	73.583	1.00	20.24	T	N
ATOM	4652	CA	PRO	T	206	33.893	19.294	74.733	1.00	21.58	T	C
ATOM	4653	C	PRO	T	206	33.465	18.464	75.947	1.00	23.90	T	C
ATOM	4654	O	PRO	T	206	32.334	17.971	75.998	1.00	23.99	T	O
ATOM	4655	CB	PRO	T	206	33.426	20.740	74.840	1.00	19.27	T	C
ATOM	4656	CG	PRO	T	206	33.146	21.107	73.403	1.00	20.23	T	C
ATOM	4657	CD	PRO	T	206	32.434	19.875	72.884	1.00	18.56	T	C
ATOM	4658	N	VAL	T	207	34.360	18.302	76.912	1.00	24.52	T	N
ATOM	4659	CA	VAL	T	207	34.052	17.528	78.109	1.00	26.63	T	C
ATOM	4660	C	VAL	T	207	33.169	18.319	79.072	1.00	28.46	T	C
ATOM	4661	O	VAL	T	207	33.402	19.499	79.320	1.00	29.61	T	O
ATOM	4662	CB	VAL	T	207	35.348	17.108	78.851	1.00	25.30	T	C
ATOM	4663	CG1	VAL	T	207	35.004	16.306	80.105	1.00	25.46	T	C
ATOM	4664	CG2	VAL	T	207	36.235	16.283	77.930	1.00	23.54	T	C
ATOM	4665	N	GLU	T	208	32.144	17.660	79.598	1.00	31.26	T	N
ATOM	4666	CA	GLU	T	208	31.231	18.269	80.556	1.00	32.65	T	C
ATOM	4667	C	GLU	T	208	31.174	17.371	81.785	1.00	34.52	T	C
ATOM	4668	O	GLU	T	208	31.032	16.161	81.662	1.00	33.84	T	O
ATOM	4669	CB	GLU	T	208	29.832	18.407	79.953	1.00	33.49	T	C
ATOM	4670	CG	GLU	T	208	29.728	19.482	78.893	1.00	37.75	T	C
ATOM	4671	CD	GLU	T	208	30.128	20.844	79.422	1.00	40.28	T	C
ATOM	4672	OE1	GLU	T	208	29.501	21.309	80.373	1.00	42.72	T	O
ATOM	4673	OE2	GLU	T	208	31.067	21.435	78.887	1.00	42.16	T	O
ATOM	4674	N	CYS	T	209	31.296	17.957	82.970	1.00	36.17	T	N
ATOM	4675	CA	CYS	T	209	31.252	17.170	84.196	1.00	38.20	T	C
ATOM	4676	C	CYS	T	209	30.084	17.610	85.068	1.00	39.82	T	C
ATOM	4677	O	CYS	T	209	29.734	18.790	85.110	1.00	39.53	T	O
ATOM	4678	CB	CYS	T	209	32.555	17.323	84.984	1.00	37.29	T	C
ATOM	4679	SG	CYS	T	209	34.098	17.006	84.069	1.00	36.18	T	S
ATOM	4680	N	MET	T	210	29.481	16.656	85.767	1.00	42.37	T	N
ATOM	4681	CA	MET	T	210	28.354	16.964	86.635	1.00	44.92	T	C
ATOM	4682	C	MET	T	210	28.859	17.451	87.987	1.00	46.67	T	C
ATOM	4683	O	MET	T	210	28.359	18.480	88.460	1.00	48.11	T	O
ATOM	4684	CB	MET	T	210	27.463	15.730	86.805	1.00	46.14	T	C
ATOM	4685	CG	MET	T	210	28.119	14.558	87.511	1.00	48.38	T	C
ATOM	4686	SD	MET	T	210	27.134	13.050	87.366	1.00	51.31	T	S
ATOM	4687	CE	MET	T	210	25.678	13.526	88.260	1.00	50.81	T	C
ATOM	4688	OT	MET	T	210	29.743	16.798	88.541	1.00	47.67	T	O
ATOM	4689	CA	CA	C	1	8.112	6.415	3.761	1.00	33.85	C	C
ATOM	4690	CA	CA	C	2	36.518	26.475	68.287	1.00	30.83	C	C
ATOM	4691	CA	CA	C	3	48.458	24.377	90.635	1.00	32.15	C	C
ATOM	4692	CA	CA	C	4	44.635	23.829	91.244	1.00	29.14	C	C
ATOM	4693	CA	CA	C	5	43.916	27.507	90.375	1.00	26.38	C	C
ATOM	4694	CA	CA	C	6	41.663	30.293	91.119	1.00	31.82	C	C
ATOM	4695	CA	CA	C	7	29.812	29.126	89.307	1.00	52.40	C	C

ATOM	4696	CA	CA	C	8	37.684	33.223	91.461	1.00	43.18	C	C
ATOM	4697	CA	CA	C	9	50.866	20.912	89.468	1.00	40.17	C	C
ATOM	4698	C11	267	I	1	35.873	7.021	10.051	1.00	13.34	I	C
ATOM	4699	O2	267	I	1	35.030	7.274	10.906	1.00	12.12	I	O
ATOM	4700	N4	267	I	1	35.755	7.412	8.778	1.00	14.34	I	N
ATOM	4701	C10	267	I	1	34.583	8.190	8.382	1.00	15.61	I	C
ATOM	4702	C13	267	I	1	34.631	8.529	6.895	1.00	13.61	I	C
ATOM	4703	C14	267	I	1	35.845	9.376	6.522	1.00	13.67	I	C
ATOM	4704	C9	267	I	1	33.296	7.419	8.715	1.00	14.50	I	C
ATOM	4705	O1	267	I	1	33.219	6.200	8.578	1.00	14.69	I	O
ATOM	4706	N3	267	I	1	32.293	8.206	9.171	1.00	12.44	I	N
ATOM	4707	C8	267	I	1	31.028	7.571	9.430	1.00	10.00	I	C
ATOM	4708	C6	267	I	1	31.561	6.344	11.579	1.00	10.55	I	C
ATOM	4709	C7	267	I	1	31.365	6.163	12.955	1.00	12.08	I	C
ATOM	4710	C2	267	I	1	30.416	6.941	13.646	1.00	12.47	I	C
ATOM	4711	C3	267	I	1	29.621	7.867	12.916	1.00	12.14	I	C
ATOM	4712	C4	267	I	1	29.820	8.053	11.556	1.00	10.96	I	C
ATOM	4713	C5	267	I	1	30.798	7.306	10.882	1.00	12.08	I	C
ATOM	4714	C1	267	I	1	30.241	6.805	15.109	1.00	12.72	I	C
ATOM	4715	N1	267	I	1	30.857	5.861	15.820	1.00	11.13	I	N
ATOM	4716	C15	267	I	1	35.718	9.758	5.051	1.00	12.95	I	C
ATOM	4717	O5	267	I	1	35.473	8.916	4.192	1.00	17.02	I	O
ATOM	4718	N6	267	I	1	35.851	11.064	4.801	1.00	14.07	I	N
ATOM	4719	C16	267	I	1	38.333	7.104	10.843	1.00	14.85	I	C
ATOM	4720	N5	267	I	1	36.894	5.189	11.391	1.00	13.27	I	N
ATOM	4721	C12	267	I	1	37.171	6.192	10.381	1.00	15.61	I	C
ATOM	4722	S1	267	I	1	36.148	3.708	10.947	1.00	18.24	I	S
ATOM	4723	O4	267	I	1	36.273	2.919	12.112	1.00	17.08	I	O
ATOM	4724	O3	267	I	1	36.874	3.315	9.787	1.00	17.15	I	O
ATOM	4725	C25	267	I	1	34.411	3.917	10.599	1.00	17.32	I	C
ATOM	4726	C26	267	I	1	33.721	2.520	10.336	1.00	16.35	I	C
ATOM	4727	N2	267	I	1	29.433	7.615	15.770	1.00	11.70	I	N
ATOM	4728	O6	267	I	1	32.719	2.228	10.988	0.00	16.69	I	O
ATOM	4729	O7	267	I	1	34.205	1.773	9.486	0.00	16.69	I	O
ATOM	4730	C21	267	I	1	41.910	4.359	13.982	0.00	15.00	I	C
ATOM	4731	C22	267	I	1	42.331	4.560	12.625	0.00	14.96	I	C
ATOM	4732	C23	267	I	1	41.530	5.218	11.673	0.00	14.93	I	C
ATOM	4733	C18	267	I	1	40.239	5.718	12.078	0.00	14.96	I	C
ATOM	4734	C19	267	I	1	39.817	5.521	13.406	0.00	14.96	I	C
ATOM	4735	C20	267	I	1	40.627	4.846	14.378	0.00	14.99	I	C
ATOM	4736	N7	267	I	1	41.683	5.545	10.332	0.00	14.91	I	N
ATOM	4737	C24	267	I	1	40.585	6.212	9.888	0.00	14.90	I	C
ATOM	4738	C17	267	I	1	39.655	6.359	10.924	0.00	15.02	I	C
ATOM	4739	OH2	WAT	W	1	9.820	12.056	12.743	1.00	14.47	W	O
ATOM	4740	OH2	WAT	W	2	21.093	10.398	10.275	1.00	7.31	W	O
ATOM	4741	OH2	WAT	W	3	32.300	19.309	24.267	1.00	9.92	W	O
ATOM	4742	OH2	WAT	W	4	24.662	17.645	24.602	1.00	12.63	W	O
ATOM	4743	OH2	WAT	W	5	10.321	9.426	13.052	1.00	13.81	W	O
ATOM	4744	OH2	WAT	W	6	12.733	19.635	-6.440	1.00	7.53	W	O
ATOM	4745	OH2	WAT	W	7	33.048	14.954	0.011	1.00	12.00	W	O
ATOM	4746	OH2	WAT	W	8	27.807	23.167	18.401	1.00	6.67	W	O
ATOM	4747	OH2	WAT	W	9	29.296	10.590	15.340	1.00	10.47	W	O
ATOM	4748	OH2	WAT	W	10	6.543	11.732	8.949	1.00	8.19	W	O
ATOM	4749	OH2	WAT	W	11	34.705	16.831	33.297	1.00	18.07	W	O
ATOM	4750	OH2	WAT	W	12	27.522	23.545	21.120	1.00	12.95	W	O
ATOM	4751	OH2	WAT	W	13	41.017	11.884	9.347	1.00	16.81	W	O

ATOM	4752	OH2	WAT	W	14	29.276	13.613	29.743	1.00	19.27	W	O
ATOM	4753	OH2	WAT	W	15	40.567	16.246	35.000	1.00	18.02	W	O
ATOM	4754	OH2	WAT	W	16	25.516	15.164	23.686	1.00	10.81	W	O
ATOM	4755	OH2	WAT	W	17	41.029	15.604	9.020	1.00	16.62	W	O
ATOM	4756	OH2	WAT	W	18	8.271	20.932	21.125	1.00	20.96	W	O
ATOM	4757	OH2	WAT	W	19	34.181	16.292	63.608	1.00	25.92	W	O
ATOM	4758	OH2	WAT	W	20	34.774	18.566	11.988	1.00	9.54	W	O
ATOM	4759	OH2	WAT	W	21	14.232	27.939	10.813	1.00	20.22	W	O
ATOM	4760	OH2	WAT	W	22	25.655	24.820	17.299	1.00	8.83	W	O
ATOM	4761	OH2	WAT	W	23	33.138	16.360	29.823	1.00	14.28	W	O
ATOM	4762	OH2	WAT	W	24	7.284	23.996	14.905	1.00	15.88	W	O
ATOM	4763	OH2	WAT	W	25	22.950	17.820	10.222	1.00	11.07	W	O
ATOM	4764	OH2	WAT	W	26	6.303	9.578	6.184	1.00	13.56	W	O
ATOM	4765	OH2	WAT	W	27	20.934	2.177	72.570	1.00	20.66	W	O
ATOM	4766	OH2	WAT	W	28	5.602	17.093	14.953	1.00	13.98	W	O
ATOM	4767	OH2	WAT	W	29	25.530	19.981	23.409	1.00	11.61	W	O
ATOM	4768	OH2	WAT	W	30	36.724	8.439	21.083	1.00	16.21	W	O
ATOM	4769	OH2	WAT	W	31	5.701	26.405	4.405	1.00	23.01	W	O
ATOM	4770	OH2	WAT	W	32	6.195	19.147	-1.275	1.00	25.93	W	O
ATOM	4771	OH2	WAT	W	33	27.238	18.873	27.707	1.00	12.95	W	O
ATOM	4772	OH2	WAT	W	34	10.019	19.300	22.404	1.00	20.89	W	O
ATOM	4773	OH2	WAT	W	35	18.660	17.642	24.646	1.00	12.31	W	O
ATOM	4774	OH2	WAT	W	36	27.000	8.766	-7.917	1.00	12.95	W	O
ATOM	4775	OH2	WAT	W	37	20.499	17.083	29.622	1.00	11.97	W	O
ATOM	4776	OH2	WAT	W	38	37.642	19.584	20.497	1.00	7.27	W	O
ATOM	4777	OH2	WAT	W	39	28.905	6.346	21.635	1.00	15.10	W	O
ATOM	4778	OH2	WAT	W	40	19.368	3.656	12.781	1.00	8.09	W	O
ATOM	4779	OH2	WAT	W	41	29.481	7.328	6.028	1.00	18.76	W	O
ATOM	4780	OH2	WAT	W	42	31.853	30.028	11.019	1.00	11.55	W	O
ATOM	4781	OH2	WAT	W	43	30.815	5.845	28.771	1.00	18.94	W	O
ATOM	4782	OH2	WAT	W	44	7.816	13.593	10.596	1.00	12.04	W	O
ATOM	4783	OH2	WAT	W	45	20.264	8.396	8.487	1.00	14.53	W	O
ATOM	4784	OH2	WAT	W	46	12.987	12.795	6.319	1.00	13.34	W	O
ATOM	4785	OH2	WAT	W	47	23.619	18.649	37.291	1.00	20.21	W	O
ATOM	4786	OH2	WAT	W	48	18.254	6.979	24.266	1.00	20.22	W	O
ATOM	4787	OH2	WAT	W	49	25.729	5.521	54.904	1.00	29.74	W	O
ATOM	4788	OH2	WAT	W	50	33.846	31.445	49.694	1.00	24.01	W	O
ATOM	4789	OH2	WAT	W	51	1.203	22.687	6.517	1.00	15.75	W	O
ATOM	4790	OH2	WAT	W	52	18.931	1.545	17.773	1.00	11.88	W	O
ATOM	4791	OH2	WAT	W	53	39.260	17.313	6.209	1.00	11.31	W	O
ATOM	4792	OH2	WAT	W	54	11.858	29.857	13.454	1.00	17.79	W	O
ATOM	4793	OH2	WAT	W	55	39.076	22.410	-1.485	1.00	9.18	W	O
ATOM	4794	OH2	WAT	W	56	26.485	33.714	15.886	1.00	19.67	W	O
ATOM	4795	OH2	WAT	W	57	37.050	20.790	0.260	1.00	15.14	W	O
ATOM	4796	OH2	WAT	W	58	27.797	26.672	32.268	1.00	28.03	W	O
ATOM	4797	OH2	WAT	W	59	18.324	13.670	16.592	1.00	14.91	W	O
ATOM	4798	OH2	WAT	W	60	17.408	28.124	11.960	1.00	22.12	W	O
ATOM	4799	OH2	WAT	W	61	30.927	20.411	26.562	1.00	11.62	W	O
ATOM	4800	OH2	WAT	W	62	9.546	29.554	23.251	1.00	25.92	W	O
ATOM	4801	OH2	WAT	W	63	19.679	15.880	80.100	1.00	32.98	W	O
ATOM	4802	OH2	WAT	W	64	32.325	25.087	22.495	1.00	35.63	W	O
ATOM	4803	OH2	WAT	W	65	30.276	24.296	21.082	1.00	13.13	W	O
ATOM	4804	OH2	WAT	W	66	13.503	-0.011	12.178	1.00	16.78	W	O
ATOM	4805	OH2	WAT	W	67	32.301	3.759	18.886	1.00	15.31	W	O
ATOM	4806	OH2	WAT	W	68	17.841	15.087	24.535	1.00	17.04	W	O
ATOM	4807	OH2	WAT	W	69	32.212	-1.864	17.231	1.00	33.57	W	O

ATOM	4808	OH2	WAT	W	70	31.942	25.422	24.949	1.00	14.32	W	0
ATOM	4809	OH2	WAT	W	71	41.741	24.676	35.656	1.00	25.77	W	0
ATOM	4810	OH2	WAT	W	72	7.065	7.005	6.381	1.00	22.12	W	0
ATOM	4811	OH2	WAT	W	73	30.082	19.209	75.060	1.00	21.78	W	0
ATOM	4812	OH2	WAT	W	74	4.031	12.254	-0.177	1.00	19.44	W	0
ATOM	4813	OH2	WAT	W	75	35.845	17.333	53.696	1.00	21.03	W	0
ATOM	4814	OH2	WAT	W	76	36.526	20.255	76.854	1.00	17.50	W	0
ATOM	4815	OH2	WAT	W	77	31.251	2.379	23.047	1.00	17.45	W	0
ATOM	4816	OH2	WAT	W	78	21.143	15.514	65.628	1.00	35.20	W	0
ATOM	4817	OH2	WAT	W	79	25.623	18.283	68.925	1.00	23.69	W	0
ATOM	4818	OH2	WAT	W	80	31.465	30.948	-2.078	1.00	41.37	W	0
ATOM	4819	OH2	WAT	W	81	24.891	29.425	38.535	1.00	32.19	W	0
ATOM	4820	OH2	WAT	W	82	26.966	27.373	47.300	1.00	31.18	W	0
ATOM	4821	OH2	WAT	W	83	29.620	34.079	-0.291	1.00	38.61	W	0
ATOM	4822	OH2	WAT	W	84	33.991	16.748	-1.768	1.00	21.41	W	0
ATOM	4823	OH2	WAT	W	85	36.100	19.081	-1.640	1.00	18.06	W	0
ATOM	4824	OH2	WAT	W	86	37.135	37.881	40.383	1.00	20.11	W	0
ATOM	4825	OH2	WAT	W	87	11.337	15.166	8.469	1.00	15.10	W	0
ATOM	4826	OH2	WAT	W	88	38.668	19.971	26.489	1.00	15.24	W	0
ATOM	4827	OH2	WAT	W	89	34.405	15.814	12.156	1.00	10.82	W	0
ATOM	4828	OH2	WAT	W	90	27.246	34.729	18.461	1.00	22.71	W	0
ATOM	4829	OH2	WAT	W	91	27.552	8.778	20.143	1.00	13.91	W	0
ATOM	4830	OH2	WAT	W	92	18.593	17.220	27.671	1.00	20.14	W	0
ATOM	4831	OH2	WAT	W	93	36.799	17.534	73.777	1.00	30.67	W	0
ATOM	4832	OH2	WAT	W	94	9.790	29.242	2.101	1.00	22.36	W	0
ATOM	4833	OH2	WAT	W	95	24.239	29.551	51.184	1.00	26.73	W	0
ATOM	4834	OH2	WAT	W	96	29.035	29.710	45.452	1.00	17.18	W	0
ATOM	4835	OH2	WAT	W	97	34.661	16.311	23.110	1.00	15.24	W	0
ATOM	4836	OH2	WAT	W	98	21.314	17.064	-7.614	1.00	27.82	W	0
ATOM	4837	OH2	WAT	W	99	30.880	19.181	28.970	1.00	18.73	W	0
ATOM	4838	OH2	WAT	W	100	28.850	17.366	29.169	1.00	18.53	W	0
ATOM	4839	OH2	WAT	W	101	42.030	21.777	13.248	1.00	26.15	W	0
ATOM	4840	OH2	WAT	W	102	3.956	12.762	-2.958	1.00	27.96	W	0
ATOM	4841	OH2	WAT	W	103	16.051	15.146	16.848	1.00	14.41	W	0
ATOM	4842	OH2	WAT	W	104	27.365	17.435	64.773	1.00	38.96	W	0
ATOM	4843	OH2	WAT	W	105	17.747	1.507	5.871	1.00	23.60	W	0
ATOM	4844	OH2	WAT	W	106	37.627	37.114	42.976	1.00	24.96	W	0
ATOM	4845	OH2	WAT	W	107	24.719	4.196	59.681	1.00	32.55	W	0
ATOM	4846	OH2	WAT	W	108	17.686	33.626	13.933	1.00	20.39	W	0
ATOM	4847	OH2	WAT	W	109	-0.184	23.823	13.296	1.00	46.49	W	0
ATOM	4848	OH2	WAT	W	110	15.373	35.019	25.333	1.00	21.46	W	0
ATOM	4849	OH2	WAT	W	111	30.768	14.093	34.177	1.00	33.90	W	0
ATOM	4850	OH2	WAT	W	112	25.218	27.843	34.700	1.00	33.99	W	0
ATOM	4851	OH2	WAT	W	113	7.403	26.902	1.736	1.00	32.04	W	0
ATOM	4852	OH2	WAT	W	114	20.038	32.869	15.272	1.00	23.28	W	0
ATOM	4853	OH2	WAT	W	115	15.360	28.092	24.066	1.00	16.94	W	0
ATOM	4854	OH2	WAT	W	116	19.926	37.657	60.577	1.00	40.46	W	0
ATOM	4855	OH2	WAT	W	117	32.502	22.719	25.889	1.00	19.53	W	0
ATOM	4856	OH2	WAT	W	118	30.616	31.722	4.387	1.00	18.60	W	0
ATOM	4857	OH2	WAT	W	119	26.479	8.176	55.645	1.00	36.63	W	0
ATOM	4858	OH2	WAT	W	120	22.372	22.465	40.919	1.00	40.52	W	0
ATOM	4859	OH2	WAT	W	121	39.623	15.685	32.220	1.00	28.34	W	0
ATOM	4860	OH2	WAT	W	122	48.066	29.461	95.001	1.00	27.75	W	0
ATOM	4861	OH2	WAT	W	123	31.897	32.419	0.487	1.00	30.32	W	0
ATOM	4862	OH2	WAT	W	124	20.734	-1.804	18.413	1.00	26.72	W	0
ATOM	4863	OH2	WAT	W	125	31.094	6.561	53.456	1.00	25.11	W	0

ATOM	4864	OH2	WAT	W	126	45.312	37.218	40.612	1.00	33.55	W	O
ATOM	4865	OH2	WAT	W	127	1.538	17.016	8.474	1.00	19.86	W	O
ATOM	4866	OH2	WAT	W	128	29.731	9.406	-1.174	1.00	20.25	W	O
ATOM	4867	OH2	WAT	W	129	27.305	38.491	25.414	1.00	28.22	W	O
ATOM	4868	OH2	WAT	W	130	28.077	29.238	30.743	1.00	23.73	W	O
ATOM	4869	OH2	WAT	W	131	26.574	28.140	51.775	1.00	15.37	W	O
ATOM	4870	OH2	WAT	W	132	19.946	5.062	76.332	1.00	36.71	W	O
ATOM	4871	OH2	WAT	W	133	10.627	12.756	10.004	1.00	22.21	W	O
ATOM	4872	OH2	WAT	W	134	11.190	-1.258	13.067	1.00	23.85	W	O
ATOM	4873	OH2	WAT	W	135	3.651	9.620	16.508	1.00	29.13	W	O
ATOM	4874	OH2	WAT	W	136	24.584	34.295	21.191	1.00	23.76	W	O
ATOM	4875	OH2	WAT	W	137	24.301	30.242	41.148	1.00	33.00	W	O
ATOM	4876	OH2	WAT	W	138	19.879	15.502	31.848	1.00	24.77	W	O
ATOM	4877	OH2	WAT	W	139	31.486	28.385	56.405	1.00	20.53	W	O
ATOM	4878	OH2	WAT	W	140	15.743	41.487	27.914	1.00	25.39	W	O
ATOM	4879	OH2	WAT	W	141	35.109	22.703	77.680	1.00	41.76	W	O
ATOM	4880	OH2	WAT	W	142	22.799	24.131	34.328	1.00	24.16	W	O
ATOM	4881	OH2	WAT	W	143	19.856	25.294	47.782	1.00	36.17	W	O
ATOM	4882	OH2	WAT	W	144	7.019	28.800	5.810	1.00	26.61	W	O
ATOM	4883	OH2	WAT	W	145	35.707	19.657	90.022	1.00	34.12	W	O
ATOM	4884	OH2	WAT	W	146	29.118	8.498	28.737	1.00	16.55	W	O
ATOM	4885	OH2	WAT	W	147	25.461	2.178	29.528	1.00	31.87	W	O
ATOM	4886	OH2	WAT	W	148	29.591	2.587	66.923	1.00	38.76	W	O
ATOM	4887	OH2	WAT	W	149	38.299	31.491	93.878	1.00	37.57	W	O
ATOM	4888	OH2	WAT	W	150	16.338	23.326	29.568	1.00	28.12	W	O
ATOM	4889	OH2	WAT	W	151	50.138	29.041	96.866	1.00	27.78	W	O
ATOM	4890	OH2	WAT	W	152	22.910	21.458	38.404	1.00	25.84	W	O
ATOM	4891	OH2	WAT	W	153	21.563	31.334	13.807	1.00	35.91	W	O
ATOM	4892	OH2	WAT	W	154	47.345	32.238	87.047	1.00	33.44	W	O
ATOM	4893	OH2	WAT	W	155	33.641	15.072	-3.898	1.00	34.95	W	O
ATOM	4894	OH2	WAT	W	156	21.869	28.002	43.965	1.00	32.96	W	O
ATOM	4895	OH2	WAT	W	157	31.608	14.352	30.918	1.00	27.70	W	O
ATOM	4896	OH2	WAT	W	158	22.471	6.040	5.325	1.00	25.62	W	O
ATOM	4897	OH2	WAT	W	159	8.576	2.761	0.289	1.00	33.92	W	O
ATOM	4898	OH2	WAT	W	160	40.895	14.749	12.622	1.00	23.15	W	O
ATOM	4899	OH2	WAT	W	161	29.005	28.427	68.038	1.00	30.48	W	O
ATOM	4900	OH2	WAT	W	162	22.507	4.454	76.352	1.00	33.53	W	O
ATOM	4901	OH2	WAT	W	163	44.106	37.763	35.688	1.00	48.32	W	O
ATOM	4902	OH2	WAT	W	164	26.450	3.355	5.768	1.00	28.13	W	O
ATOM	4903	OH2	WAT	W	165	4.723	30.331	5.955	1.00	44.11	W	O
ATOM	4904	OH2	WAT	W	166	35.185	27.903	-4.961	1.00	27.15	W	O
ATOM	4905	OH2	WAT	W	167	18.473	10.311	-5.754	1.00	31.75	W	O
ATOM	4906	OH2	WAT	W	168	31.008	4.482	21.032	1.00	44.53	W	O
ATOM	4907	OH2	WAT	W	169	38.894	15.944	48.372	1.00	38.35	W	O
ATOM	4908	OH2	WAT	W	170	34.331	25.697	20.938	1.00	21.61	W	O
ATOM	4909	OH2	WAT	W	171	49.199	26.268	86.643	1.00	30.58	W	O
ATOM	4910	OH2	WAT	W	172	5.127	9.693	-0.969	1.00	34.66	W	O
ATOM	4911	OH2	WAT	W	173	-0.373	13.989	8.086	1.00	34.97	W	O
ATOM	4912	OH2	WAT	W	174	16.470	-0.001	3.800	1.00	32.29	W	O
ATOM	4913	OH2	WAT	W	175	18.074	31.513	1.418	1.00	34.23	W	O
ATOM	4914	OH2	WAT	W	176	38.094	40.562	31.950	1.00	29.70	W	O
ATOM	4915	OH2	WAT	W	177	40.881	31.784	48.268	1.00	38.43	W	O
ATOM	4916	OH2	WAT	W	178	33.053	31.307	3.076	1.00	21.18	W	O
ATOM	4917	OH2	WAT	W	179	5.567	14.818	-1.815	1.00	30.86	W	O
ATOM	4918	OH2	WAT	W	180	31.429	9.957	46.073	1.00	34.20	W	O
ATOM	4919	OH2	WAT	W	181	11.917	28.333	8.565	1.00	16.99	W	O

ATOM	4920	OH2	WAT	W	182	36.688	10.228	42.234	1.00	32.93	W	0
ATOM	4921	OH2	WAT	W	183	3.251	31.546	9.757	1.00	29.65	W	0
ATOM	4922	OH2	WAT	W	184	18.321	2.574	-0.484	1.00	32.80	W	0
ATOM	4923	OH2	WAT	W	185	5.637	5.762	14.955	1.00	32.54	W	0
ATOM	4924	OH2	WAT	W	186	15.673	14.210	25.757	1.00	34.67	W	0
ATOM	4925	OH2	WAT	W	187	40.626	21.784	27.626	1.00	32.36	W	0
ATOM	4926	OH2	WAT	W	188	42.987	22.261	89.602	1.00	27.87	W	0
ATOM	4927	OH2	WAT	W	189	14.638	39.203	19.516	1.00	32.86	W	0
ATOM	4928	OH2	WAT	W	190	11.036	30.934	11.072	1.00	31.17	W	0
ATOM	4929	OH2	WAT	W	191	33.710	31.642	9.747	1.00	31.14	W	0
ATOM	4930	OH2	WAT	W	192	20.870	6.918	26.506	1.00	33.93	W	0
ATOM	4931	OH2	WAT	W	193	28.954	1.020	74.566	1.00	34.78	W	0
ATOM	4932	OH2	WAT	W	194	37.700	14.002	57.999	1.00	52.48	W	0
ATOM	4933	OH2	WAT	W	195	2.310	11.077	13.236	1.00	36.20	W	0
ATOM	4934	OH2	WAT	W	196	29.084	-0.199	11.021	1.00	39.14	W	0
ATOM	4935	OH2	WAT	W	197	41.032	19.200	6.700	1.00	29.69	W	0
ATOM	4936	OH2	WAT	W	198	12.343	28.516	23.498	1.00	25.52	W	0
ATOM	4937	OH2	WAT	W	199	28.735	31.233	43.028	1.00	25.67	W	0
ATOM	4938	OH2	WAT	W	200	44.326	3.129	25.867	1.00	53.38	W	0
ATOM	4939	OH2	WAT	W	201	28.603	7.431	-2.611	1.00	30.58	W	0
ATOM	4940	OH2	WAT	W	202	33.156	26.217	56.692	1.00	26.48	W	0
ATOM	4941	OH2	WAT	W	203	36.278	15.450	-4.311	1.00	26.09	W	0
ATOM	4942	OH2	WAT	W	204	38.154	8.018	19.062	1.00	37.43	W	0
ATOM	4943	OH2	WAT	W	205	9.837	28.610	10.272	1.00	31.67	W	0
ATOM	4944	OH2	WAT	W	206	14.373	16.403	26.718	1.00	36.07	W	0
ATOM	4945	OH2	WAT	W	207	37.593	16.593	70.391	1.00	29.23	W	0
ATOM	4946	OH2	WAT	W	208	0.132	11.716	9.251	1.00	33.00	W	0
ATOM	4947	OH2	WAT	W	209	25.144	28.339	31.889	1.00	49.28	W	0
ATOM	4948	OH2	WAT	W	210	7.440	16.389	-2.874	1.00	20.15	W	0
ATOM	4949	OH2	WAT	W	211	7.530	29.833	8.482	1.00	30.21	W	0
ATOM	4950	OH2	WAT	W	212	21.589	17.888	38.999	1.00	33.78	W	0
ATOM	4951	OH2	WAT	W	213	42.227	19.920	8.912	1.00	24.14	W	0
ATOM	4952	OH2	WAT	W	214	18.081	13.134	53.952	1.00	46.05	W	0
ATOM	4953	OH2	WAT	W	215	28.604	36.515	31.266	1.00	35.94	W	0
ATOM	4954	OH2	WAT	W	216	21.979	38.636	47.184	1.00	45.57	W	0
ATOM	4955	OH2	WAT	W	217	37.628	28.720	13.544	1.00	35.13	W	0
ATOM	4956	OH2	WAT	W	218	13.553	15.154	18.167	1.00	30.54	W	0
ATOM	4957	OH2	WAT	W	219	32.654	30.845	47.076	1.00	25.26	W	0
ATOM	4958	OH2	WAT	W	220	-2.842	14.831	8.115	1.00	33.07	W	0
ATOM	4959	OH2	WAT	W	221	18.483	15.571	-7.984	1.00	30.86	W	0
ATOM	4960	OH2	WAT	W	222	3.270	25.714	5.665	1.00	26.54	W	0
ATOM	4961	OH2	WAT	W	223	50.144	24.757	82.596	1.00	34.50	W	0
ATOM	4962	OH2	WAT	W	224	26.242	11.203	31.526	1.00	30.44	W	0
ATOM	4963	OH2	WAT	W	225	18.073	-1.159	18.149	1.00	34.58	W	0
ATOM	4964	OH2	WAT	W	226	47.321	29.376	85.710	1.00	34.51	W	0
ATOM	4965	OH2	WAT	W	227	22.195	20.381	42.496	1.00	30.12	W	0
ATOM	4966	OH2	WAT	W	228	3.659	2.259	0.190	1.00	34.67	W	0
ATOM	4967	OH2	WAT	W	229	40.557	0.237	20.769	1.00	28.72	W	0
ATOM	4968	OH2	WAT	W	230	21.900	26.386	53.079	1.00	26.13	W	0
ATOM	4969	OH2	WAT	W	231	7.647	31.085	26.330	1.00	35.78	W	0
ATOM	4970	OH2	WAT	W	232	13.007	21.995	27.742	1.00	38.60	W	0
ATOM	4971	OH2	WAT	W	233	45.245	0.872	24.555	1.00	46.33	W	0
ATOM	4972	OH2	WAT	W	234	18.696	16.785	50.319	1.00	37.87	W	0
ATOM	4973	OH2	WAT	W	235	31.471	4.379	68.498	1.00	43.22	W	0
ATOM	4974	OH2	WAT	W	236	44.018	19.076	33.450	1.00	32.66	W	0
ATOM	4975	OH2	WAT	W	237	23.071	24.930	30.360	1.00	23.93	W	0

ATOM	4976	OH2	WAT	W	238	35.628	33.217	93.628	1.00	33.30	W	0
ATOM	4977	OH2	WAT	W	239	35.847	25.095	70.900	1.00	44.01	W	0
ATOM	4978	OH2	WAT	W	240	22.701	20.328	82.692	1.00	39.98	W	0
ATOM	4979	OH2	WAT	W	241	7.838	12.303	-1.787	1.00	34.86	W	0
ATOM	4980	OH2	WAT	W	242	28.268	21.326	68.248	1.00	31.86	W	0
ATOM	4981	OH2	WAT	W	243	-0.770	24.146	8.061	1.00	34.90	W	0
ATOM	4982	OH2	WAT	W	244	38.119	6.075	7.064	1.00	31.06	W	0
ATOM	4983	OH2	WAT	W	245	23.502	28.608	54.003	1.00	28.10	W	0
ATOM	4984	OH2	WAT	W	246	34.476	12.129	8.573	1.00	22.78	W	0
ATOM	4985	OH2	WAT	W	247	11.730	40.646	20.091	1.00	43.62	W	0
ATOM	4986	OH2	WAT	W	248	20.358	23.090	67.179	1.00	43.07	W	0
ATOM	4987	OH2	WAT	W	249	33.233	30.859	32.765	1.00	29.52	W	0
ATOM	4988	OH2	WAT	W	250	34.971	29.300	13.451	1.00	24.97	W	0
ATOM	4989	OH2	WAT	W	251	21.456	30.121	50.897	1.00	51.79	W	0
ATOM	4990	OH2	WAT	W	252	38.432	11.736	55.327	1.00	41.69	W	0
ATOM	4991	OH2	WAT	W	253	42.192	23.969	9.558	1.00	58.78	W	0
ATOM	4992	OH2	WAT	W	254	45.254	27.469	47.916	1.00	33.81	W	0
ATOM	4993	OH2	WAT	W	255	34.867	39.746	60.424	1.00	51.82	W	0
ATOM	4994	OH2	WAT	W	256	7.714	11.590	23.225	1.00	47.38	W	0
ATOM	4995	OH2	WAT	W	257	11.234	37.040	13.444	1.00	45.19	W	0
ATOM	4996	OH2	WAT	W	258	5.250	24.259	16.611	1.00	35.12	W	0
ATOM	4997	OH2	WAT	W	259	30.634	7.333	46.566	1.00	64.60	W	0
ATOM	4998	OH2	WAT	W	260	41.043	28.449	49.954	1.00	34.29	W	0
ATOM	4999	OH2	WAT	W	261	27.833	42.178	56.031	1.00	38.43	W	0
ATOM	5000	OH2	WAT	W	262	36.007	23.861	20.102	1.00	26.54	W	0
ATOM	5001	OH2	WAT	W	263	47.752	24.361	74.233	1.00	52.97	W	0
ATOM	5002	OH2	WAT	W	264	20.405	19.480	-9.352	1.00	39.53	W	0
ATOM	5003	OH2	WAT	W	265	27.553	31.025	88.317	1.00	52.14	W	0
ATOM	5004	OH2	WAT	W	266	27.439	6.871	2.671	1.00	33.49	W	0
ATOM	5005	OH2	WAT	W	267	28.522	39.164	45.564	1.00	34.68	W	0
ATOM	5006	OH2	WAT	W	268	43.870	22.301	47.233	1.00	40.78	W	0
ATOM	5007	OH2	WAT	W	269	35.079	36.340	52.168	1.00	44.82	W	0
ATOM	5008	OH2	WAT	W	270	23.451	34.163	23.718	1.00	27.05	W	0
ATOM	5009	OH2	WAT	W	271	30.957	22.554	71.076	1.00	42.91	W	0
ATOM	5010	OH2	WAT	W	272	38.744	7.564	80.920	1.00	40.95	W	0
ATOM	5011	OH2	WAT	W	273	13.936	30.988	30.446	1.00	41.06	W	0
ATOM	5012	OH2	WAT	W	274	23.419	17.708	86.267	1.00	59.87	W	0
ATOM	5013	OH2	WAT	W	275	21.017	0.277	3.695	1.00	50.07	W	0
ATOM	5014	OH2	WAT	W	276	21.549	22.757	36.427	1.00	45.15	W	0
ATOM	5015	OH2	WAT	W	277	37.355	12.567	39.061	1.00	34.74	W	0
ATOM	5016	OH2	WAT	W	278	2.783	23.907	15.169	1.00	48.05	W	0
ATOM	5017	OH2	WAT	W	279	32.292	35.378	41.347	1.00	45.51	W	0
ATOM	5018	OH2	WAT	W	280	24.285	8.129	48.241	1.00	36.55	W	0
ATOM	5019	OH2	WAT	W	281	9.135	10.036	-0.985	1.00	36.77	W	0
ATOM	5020	OH2	WAT	W	282	9.648	4.536	20.435	1.00	35.26	W	0
ATOM	5021	OH2	WAT	W	283	37.143	14.114	86.099	1.00	40.95	W	0
ATOM	5022	OH2	WAT	W	284	9.020	35.287	33.571	1.00	41.52	W	0
ATOM	5023	OH2	WAT	W	285	-1.612	10.514	3.421	1.00	51.73	W	0
ATOM	5024	OH2	WAT	W	286	42.982	17.337	41.377	1.00	38.67	W	0
ATOM	5025	OH2	WAT	W	287	34.957	31.854	45.389	1.00	25.75	W	0
ATOM	5026	OH2	WAT	W	288	3.170	28.704	16.548	1.00	47.39	W	0
ATOM	5027	OH2	WAT	W	289	4.236	26.437	18.194	1.00	40.60	W	0
ATOM	5028	OH2	WAT	W	290	11.780	0.909	19.173	1.00	31.13	W	0
ATOM	5029	OH2	WAT	W	291	35.076	18.990	60.316	1.00	38.09	W	0
ATOM	5030	OH2	WAT	W	292	-0.662	15.295	21.926	1.00	52.48	W	0
ATOM	5031	OH2	WAT	W	293	42.355	22.441	69.467	1.00	43.05	W	0

ATOM	5032	OH2	WAT	W	294	36.115	8.550	0.838	1.00	34.86	W	0
ATOM	5033	OH2	WAT	W	295	5.539	38.578	29.277	1.00	41.01	W	0
ATOM	5034	OH2	WAT	W	296	-0.774	16.342	12.374	1.00	44.15	W	0
ATOM	5035	OH2	WAT	W	297	20.248	19.074	34.881	1.00	32.03	W	0
ATOM	5036	OH2	WAT	W	298	22.485	11.810	37.890	1.00	40.55	W	0
ATOM	5037	OH2	WAT	W	299	42.707	16.687	11.459	1.00	42.38	W	0
ATOM	5038	OH2	WAT	W	300	40.839	15.634	41.011	1.00	38.21	W	0
ATOM	5039	OH2	WAT	W	301	20.094	24.068	71.878	1.00	70.09	W	0
ATOM	5040	OH2	WAT	W	302	31.865	-0.414	10.192	1.00	41.10	W	0
ATOM	5041	OH2	WAT	W	303	20.743	26.537	50.189	1.00	45.73	W	0
ATOM	5042	OH2	WAT	W	304	44.143	13.662	12.378	1.00	40.41	W	0
ATOM	5043	OH2	WAT	W	305	40.498	25.176	54.332	1.00	46.48	W	0
ATOM	5044	OH2	WAT	W	306	35.746	6.890	18.386	1.00	32.88	W	0
ATOM	5045	OH2	WAT	W	307	14.855	41.757	31.970	1.00	44.75	W	0
ATOM	5046	OH2	WAT	W	308	18.143	-0.909	20.903	1.00	45.80	W	0
ATOM	5047	OH2	WAT	W	309	27.593	7.517	-5.357	1.00	51.75	W	0
ATOM	5048	OH2	WAT	W	310	29.441	20.038	-9.566	1.00	48.48	W	0
ATOM	5049	OH2	WAT	W	311	33.031	8.376	2.930	1.00	37.72	W	0
ATOM	5050	OH2	WAT	W	312	28.826	12.995	39.392	1.00	28.46	W	0
ATOM	5051	OH2	WAT	W	313	19.453	26.455	33.576	1.00	49.37	W	0
ATOM	5052	OH2	WAT	W	314	32.900	12.710	60.296	1.00	43.04	W	0
ATOM	5053	OH2	WAT	W	315	35.171	34.093	47.106	1.00	46.97	W	0
ATOM	5054	OH2	WAT	W	316	42.577	27.086	48.235	1.00	40.03	W	0
ATOM	5055	OH2	WAT	W	317	8.900	30.335	4.530	1.00	36.15	W	0
ATOM	5056	OH2	WAT	W	318	30.817	33.985	69.076	1.00	46.39	W	0
ATOM	5057	OH2	WAT	W	319	19.929	3.244	55.862	1.00	64.48	W	0
ATOM	5058	OH2	WAT	W	320	23.376	1.981	90.249	1.00	39.58	W	0
ATOM	5059	OH2	WAT	W	321	40.437	5.728	17.654	1.00	39.03	W	0
ATOM	5060	OH2	WAT	W	322	9.640	35.993	11.234	1.00	42.42	W	0
ATOM	5061	OH2	WAT	W	323	16.153	42.346	23.466	1.00	34.97	W	0
ATOM	5062	OH2	WAT	W	324	35.436	19.673	64.215	1.00	57.86	W	0
ATOM	5063	OH2	WAT	W	325	4.918	16.942	5.288	1.00	10.46	W	0
ATOM	5064	OH2	WAT	W	326	18.390	21.278	-9.254	1.00	31.50	W	0
ATOM	5065	OH2	WAT	W	327	1.490	16.464	5.809	1.00	20.84	W	0
ATOM	5066	OH2	WAT	W	328	2.997	16.779	3.328	1.00	19.39	W	0
ATOM	5067	OH2	WAT	W	329	6.139	1.050	-0.292	1.00	48.96	W	0
ATOM	5068	OH2	WAT	W	330	35.510	12.689	47.619	1.00	31.05	W	0
ATOM	5069	OH2	WAT	W	331	27.536	5.618	-0.676	1.00	54.07	W	0
ATOM	5070	OH2	WAT	W	332	43.643	19.826	17.185	1.00	59.51	W	0
ATOM	5071	OH2	WAT	W	333	19.184	30.073	10.467	1.00	46.29	W	0
ATOM	5072	OH2	WAT	W	334	31.305	28.910	32.552	1.00	37.09	W	0
ATOM	5073	OH2	WAT	W	335	9.970	0.903	-1.332	1.00	48.94	W	0
ATOM	5074	OH2	WAT	W	336	42.603	21.451	5.443	1.00	46.05	W	0
ATOM	5075	OH2	WAT	W	337	25.589	37.355	19.101	1.00	50.70	W	0
ATOM	5076	OH2	WAT	W	338	16.211	15.273	77.481	1.00	45.46	W	0
ATOM	5077	OH2	WAT	W	339	4.566	4.778	9.222	1.00	38.03	W	0
ATOM	5078	OH2	WAT	W	340	24.583	13.388	-12.370	1.00	38.31	W	0
ATOM	5079	OH2	WAT	W	341	41.377	15.443	47.138	1.00	42.95	W	0
ATOM	5080	OH2	WAT	W	342	46.584	22.712	72.438	1.00	50.39	W	0
ATOM	5081	OH2	WAT	W	343	37.742	-1.808	21.784	1.00	43.11	W	0
ATOM	5082	OH2	WAT	W	344	19.595	0.633	24.707	1.00	42.68	W	0
ATOM	5083	OH2	WAT	W	345	20.648	23.506	31.934	1.00	41.44	W	0
ATOM	5084	OH2	WAT	W	346	5.215	28.843	9.509	1.00	27.51	W	0
ATOM	5085	OH2	WAT	W	347	-1.391	17.437	9.148	1.00	44.39	W	0
ATOM	5086	OH2	WAT	W	348	37.699	11.902	32.487	1.00	31.25	W	0
ATOM	5087	OH2	WAT	W	349	21.639	34.577	35.581	1.00	39.86	W	0

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ATOM   5088  OH2 WAT W 350      19.819  24.919  38.691  1.00 51.89      W    O
ATOM   5089  OH2 WAT W 351      34.940  35.726  43.895  1.00 60.97      W    O
ATOM   5090  OH2 WAT W 352      37.201  17.622  58.850  1.00 43.91      W    O
ATOM   5091  OH2 WAT W 353      29.384  35.815  62.018  1.00 33.90      W    O
ATOM   5092  OH2 WAT W 354      34.042  37.937  56.652  1.00 31.53      W    O
ATOM   5093  OH2 WAT W 355      18.864  -1.487   3.101  1.00 49.21      W    O
ATOM   5094  OH2 WAT W 356      45.897  16.661  41.685  1.00 45.52      W    O
ATOM   5095  OH2 WAT W 357      46.644  36.386  90.281  1.00 51.76      W    O
ATOM   5096  OH2 WAT W 358      25.350  25.538  31.973  1.00 43.63      W    O
ATOM   5097  OH2 WAT W 359      34.925   5.802  29.713  1.00 38.77      W    O
ATOM   5098  OH2 WAT W 360      33.389  12.245  -5.833  1.00 38.52      W    O
ATOM   5099  OH2 WAT W 361      13.401  36.615   6.966  1.00 60.27      W    O
ATOM   5100  OH2 WAT W 362      29.038  14.217  36.874  1.00 43.15      W    O
ATOM   5101  OH2 WAT W 363      43.754  18.992  93.095  1.00 43.98      W    O
ATOM   5102  OH2 WAT W 364      24.549   4.764   4.197  1.00 50.16      W    O
ATOM   5103  OH2 WAT W 365      43.227  13.919  19.497  1.00 58.10      W    O
ATOM   5104  OH2 WAT W 366      10.214  33.407   9.945  1.00 50.53      W    O
ATOM   5105  OH2 WAT W 367      17.413  19.604  27.704  1.00 31.46      W    O
ATOM   5106  OH2 WAT W 368      28.562  31.651  91.027  1.00 58.48      W    O
ATOM   5107  OH2 WAT W 369      39.915   9.085   8.229  1.00 51.34      W    O
ATOM   5108  OH2 WAT W 370      37.715   6.403   1.728  1.00 49.76      W    O
ATOM   5109  OH2 WAT W 371      45.177  11.389  17.053  1.00 38.62      W    O
ATOM   5110  OH2 WAT W 372      -1.495  16.407   5.919  1.00 24.58      W    O
ATOM   5111  OH2 WAT W 373      17.928  10.777  -8.990  1.00 48.78      W    O
ATOM   5112  OH2 WAT W 374      49.671  41.399  35.418  1.00 39.49      W    O
ATOM   5113  OH2 WAT W 375      -2.896  22.960   9.444  1.00 64.43      W    O
ATOM   5114  OH2 WAT W 376      44.242  20.119  13.114  1.00 43.91      W    O
ATOM   5115  OH2 WAT W 377      45.998  27.498  65.911  1.00 52.62      W    O
ATOM   5116  OH2 WAT W 378      54.712  25.922  87.283  1.00 44.48      W    O
ATOM   5117  OH2 WAT W 379       9.336  21.221  24.256  1.00 39.28      W    O
ATOM   5118  OH2 WAT W 380       5.711  10.622  25.188  1.00 45.01      W    O
ATOM   5119  OH2 WAT W 381      22.065  36.408  12.747  1.00 59.06      W    O
ATOM   5120  OH2 WAT W 382      16.957  10.821  43.808  1.00 40.75      W    O
ATOM   5121  OH2 WAT W 383      39.595   1.633  12.436  1.00 49.31      W    O
ATOM   5122  OH2 WAT W 384      11.084  30.834   0.209  1.00 39.09      W    O
ATOM   5123  OH2 WAT W 385      16.720  27.264  -4.002  1.00 41.06      W    O
ATOM   5124  OH2 WAT W 386      31.056   0.281  79.010  1.00 38.99      W    O
ATOM   5125  OH2 WAT W 387      19.887   9.930  45.039  1.00 49.86      W    O
ATOM   5126  OH2 WAT W 388      36.655  37.162  45.509  1.00 47.87      W    O
ATOM   5127  OH2 WAT W 389      27.630   7.903  30.948  1.00 41.08      W    O
ATOM   5128  OH2 WAT W 390      22.128  23.087  -9.666  1.00 41.60      W    O
ATOM   5129  OH2 WAT W 391      16.596  34.405   7.509  1.00 52.09      W    O
ATOM   5130  OH2 WAT W 392      18.187  37.051  16.426  1.00 58.25      W    O
ATOM   5131  OH2 WAT W 393      20.557  35.471  15.670  1.00 30.35      W    O
ATOM   5132  OH2 WAT W 394      38.852  10.942  68.815  1.00 56.37      W    O
ATOM   5133  OH2 WAT W 395      14.789  20.103  63.603  1.00 69.08      W    O
ATOM   5134  OH2 WAT W 396      35.781   9.917  61.122  1.00 45.92      W    O
ATOM   5135  OH2 WAT W 397      32.425   7.986  44.362  1.00 50.04      W    O
ATOM   5136  OH2 WAT W 398      39.173  29.239  58.940  1.00 46.65      W    O
ATOM   5137  OH2 WAT W 399      33.925  28.356  71.709  1.00 46.27      W    O
ATOM   5138  OH2 WAT W 400      26.195  11.085  39.837  1.00 37.48      W    O
ATOM   5139  OH2 WAT W 401      40.425   2.450   9.983  1.00 44.75      W    O
ATOM   5140  OH2 WAT W 402      28.452  -1.394   7.667  1.00 56.86      W    O
ATOM   5141  OH2 WAT W 403      22.460   2.393   0.537  1.00 46.38      W    O
ATOM   5142  OH2 WAT W 404      20.613   0.672  -0.814  1.00 61.12      W    O
END
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Table 37 Coordinate data of the complex between Compound (2) and human factor VIIa/soluble tissue factor (around the inhibitor)

CRYST1	71.280	82.320	123.380	90.00	90.00	90.00	P212121					
ATOM	1	N	ILE	H	16	22.059	3.893	14.020	1.00	5.70	H	N
ATOM	2	CA	ILE	H	16	21.957	4.124	15.491	1.00	6.52	H	C
ATOM	3	C	ILE	H	16	22.005	2.782	16.220	1.00	7.66	H	C
ATOM	4	O	ILE	H	16	21.209	1.883	15.942	1.00	8.62	H	O
ATOM	5	CB	ILE	H	16	20.628	4.834	15.856	1.00	7.20	H	C
ATOM	6	CG1	ILE	H	16	20.515	6.174	15.119	1.00	6.97	H	C
ATOM	7	CG2	ILE	H	16	20.545	5.036	17.365	1.00	7.03	H	C
ATOM	8	CD1	ILE	H	16	21.554	7.217	15.521	1.00	6.54	H	C
ATOM	9	N	VAL	H	17	22.947	2.646	17.144	1.00	8.63	H	N
ATOM	10	CA	VAL	H	17	23.087	1.417	17.916	1.00	9.50	H	C
ATOM	11	C	VAL	H	17	22.570	1.634	19.338	1.00	9.85	H	C
ATOM	12	O	VAL	H	17	23.002	2.553	20.026	1.00	10.72	H	O
ATOM	13	CB	VAL	H	17	24.566	0.964	18.008	1.00	9.85	H	C
ATOM	14	CG1	VAL	H	17	24.659	-0.327	18.813	1.00	10.27	H	C
ATOM	15	CG2	VAL	H	17	25.148	0.754	16.613	1.00	9.47	H	C
ATOM	16	N	LEU	H	41	22.072	7.406	1.097	1.00	11.66	H	N
ATOM	17	CA	LEU	H	41	23.440	7.899	1.213	1.00	11.08	H	C
ATOM	18	C	LEU	H	41	23.808	8.366	2.624	1.00	10.34	H	C
ATOM	19	O	LEU	H	41	24.765	7.871	3.224	1.00	10.61	H	O
ATOM	20	CB	LEU	H	41	23.657	9.058	0.226	1.00	10.87	H	C
ATOM	21	CG	LEU	H	41	25.000	9.801	0.273	1.00	11.44	H	C
ATOM	22	CD1	LEU	H	41	26.115	8.893	-0.221	1.00	11.67	H	C
ATOM	23	CD2	LEU	H	41	24.921	11.048	-0.582	1.00	11.04	H	C
ATOM	24	N	CYS	H	42	23.032	9.307	3.153	1.00	8.47	H	N
ATOM	25	CA	CYS	H	42	23.314	9.885	4.457	1.00	6.60	H	C
ATOM	26	C	CYS	H	42	22.102	10.577	5.061	1.00	6.35	H	C
ATOM	27	O	CYS	H	42	21.038	10.660	4.448	1.00	8.53	H	O
ATOM	28	CB	CYS	H	42	24.421	10.935	4.309	1.00	6.00	H	C
ATOM	29	SG	CYS	H	42	26.138	10.338	4.348	1.00	7.26	H	S
ATOM	30	N	GLY	H	43	22.291	11.087	6.272	1.00	4.57	H	N
ATOM	31	CA	GLY	H	43	21.248	11.827	6.949	1.00	3.67	H	C
ATOM	32	C	GLY	H	43	21.549	13.308	6.764	1.00	3.89	H	C
ATOM	33	O	GLY	H	43	22.525	13.686	6.104	1.00	3.23	H	O
ATOM	34	N	ALA	H	55	26.992	16.158	6.411	1.00	5.39	H	N
ATOM	35	CA	ALA	H	55	28.424	15.958	6.611	1.00	5.45	H	C
ATOM	36	C	ALA	H	55	29.160	15.980	5.277	1.00	6.95	H	C
ATOM	37	O	ALA	H	55	28.674	15.441	4.279	1.00	6.34	H	O
ATOM	38	CB	ALA	H	55	28.681	14.624	7.326	1.00	4.19	H	C
ATOM	39	N	ALA	H	56	30.333	16.606	5.265	1.00	6.14	H	N
ATOM	40	CA	ALA	H	56	31.142	16.694	4.053	1.00	7.74	H	C
ATOM	41	C	ALA	H	56	31.552	15.332	3.488	1.00	6.96	H	C
ATOM	42	O	ALA	H	56	31.487	15.118	2.276	1.00	8.41	H	O
ATOM	43	CB	ALA	H	56	32.399	17.532	4.319	1.00	6.48	H	C
ATOM	44	N	HIS	H	57	31.971	14.412	4.355	1.00	5.95	H	N
ATOM	45	CA	HIS	H	57	32.419	13.103	3.889	1.00	6.77	H	C
ATOM	46	C	HIS	H	57	31.358	12.282	3.151	1.00	8.28	H	C
ATOM	47	O	HIS	H	57	31.685	11.304	2.476	1.00	8.26	H	O
ATOM	48	CB	HIS	H	57	33.021	12.288	5.046	1.00	5.22	H	C

ATOM	49	CG	HIS	H	57	32.022	11.512	5.846	1.00	4.67	H	C
ATOM	50	ND1	HIS	H	57	31.558	11.936	7.074	1.00	2.15	H	N
ATOM	51	CD2	HIS	H	57	31.432	10.314	5.613	1.00	3.66	H	C
ATOM	52	CE1	HIS	H	57	30.730	11.032	7.564	1.00	2.30	H	C
ATOM	53	NE2	HIS	H	57	30.636	10.038	6.698	1.00	3.94	H	N
ATOM	54	N	CYS	H	58	30.096	12.686	3.267	1.00	7.28	H	N
ATOM	55	CA	CYS	H	58	29.008	11.999	2.584	1.00	8.91	H	C
ATOM	56	C	CYS	H	58	29.128	12.140	1.069	1.00	9.73	H	C
ATOM	57	O	CYS	H	58	28.496	11.407	0.317	1.00	7.76	H	O
ATOM	58	CB	CYS	H	58	27.660	12.578	3.035	1.00	7.86	H	C
ATOM	59	SG	CYS	H	58	27.176	12.043	4.706	1.00	6.38	H	S
ATOM	60	N	PHE	H	59	29.962	13.074	0.628	1.00	10.76	H	N
ATOM	61	CA	PHE	H	59	30.114	13.347	-0.790	1.00	9.91	H	C
ATOM	62	C	PHE	H	59	31.481	12.971	-1.364	1.00	9.71	H	C
ATOM	63	O	PHE	H	59	31.804	13.337	-2.496	1.00	8.14	H	O
ATOM	64	CB	PHE	H	59	29.804	14.832	-1.020	1.00	9.77	H	C
ATOM	65	CG	PHE	H	59	28.484	15.267	-0.422	1.00	10.32	H	C
ATOM	66	CD1	PHE	H	59	27.287	15.011	-1.083	1.00	7.39	H	C
ATOM	67	CD2	PHE	H	59	28.436	15.845	0.846	1.00	11.05	H	C
ATOM	68	CE1	PHE	H	59	26.061	15.314	-0.493	1.00	9.49	H	C
ATOM	69	CE2	PHE	H	59	27.214	16.151	1.447	1.00	11.89	H	C
ATOM	70	CZ	PHE	H	59	26.023	15.884	0.776	1.00	10.25	H	C
ATOM	71	N	ASP	H	60	32.273	12.230	-0.591	1.00	8.71	H	N
ATOM	72	CA	ASP	H	60	33.596	11.796	-1.041	1.00	11.41	H	C
ATOM	73	C	ASP	H	60	33.570	11.036	-2.370	1.00	13.85	H	C
ATOM	74	O	ASP	H	60	34.394	11.286	-3.250	1.00	13.33	H	O
ATOM	75	CB	ASP	H	60	34.255	10.904	0.016	1.00	9.72	H	C
ATOM	76	CG	ASP	H	60	34.855	11.694	1.157	1.00	10.46	H	C
ATOM	77	OD1	ASP	H	60	34.672	12.930	1.191	1.00	8.35	H	O
ATOM	78	OD2	ASP	H	60	35.514	11.074	2.020	1.00	9.24	H	O
ATOM	79	N	LYS	H	60A	32.634	10.105	-2.522	1.00	15.64	H	N
ATOM	80	CA	LYS	H	60A	32.579	9.330	-3.755	1.00	19.34	H	C
ATOM	81	C	LYS	H	60A	31.407	9.614	-4.690	1.00	19.44	H	C
ATOM	82	O	LYS	H	60A	30.971	8.728	-5.420	1.00	19.48	H	O
ATOM	83	CB	LYS	H	60A	32.624	7.830	-3.441	1.00	21.25	H	C
ATOM	84	CG	LYS	H	60A	34.024	7.315	-3.136	1.00	25.19	H	C
ATOM	85	CD	LYS	H	60A	34.292	7.216	-1.650	1.00	28.66	H	C
ATOM	86	CE	LYS	H	60A	33.594	6.006	-1.041	1.00	31.51	H	C
ATOM	87	NZ	LYS	H	60A	33.915	5.848	0.412	1.00	35.53	H	N
ATOM	88	N	ILE	H	90	30.977	22.763	0.695	1.00	7.99	H	N
ATOM	89	CA	ILE	H	90	31.915	22.141	1.623	1.00	7.65	H	C
ATOM	90	C	ILE	H	90	33.092	23.074	1.866	1.00	7.29	H	C
ATOM	91	O	ILE	H	90	33.544	23.761	0.953	1.00	9.45	H	O
ATOM	92	CB	ILE	H	90	32.422	20.804	1.016	1.00	7.65	H	C
ATOM	93	CG1	ILE	H	90	31.298	19.767	1.061	1.00	8.19	H	C
ATOM	94	CG2	ILE	H	90	33.667	20.313	1.732	1.00	8.25	H	C
ATOM	95	CD1	ILE	H	90	31.620	18.477	0.319	1.00	9.60	H	C
ATOM	96	N	TYR	H	94	38.317	21.049	3.982	1.00	8.73	H	N
ATOM	97	CA	TYR	H	94	37.972	19.637	4.148	1.00	7.55	H	C
ATOM	98	C	TYR	H	94	38.721	18.785	3.130	1.00	7.26	H	C
ATOM	99	O	TYR	H	94	38.805	19.138	1.959	1.00	6.40	H	O
ATOM	100	CB	TYR	H	94	36.464	19.404	3.969	1.00	5.85	H	C
ATOM	101	CG	TYR	H	94	36.110	17.927	3.920	1.00	4.59	H	C
ATOM	102	CD1	TYR	H	94	36.088	17.157	5.082	1.00	4.45	H	C
ATOM	103	CD2	TYR	H	94	35.884	17.281	2.700	1.00	4.26	H	C
ATOM	104	CE1	TYR	H	94	35.859	15.780	5.035	1.00	2.80	H	C

ATOM	105	CE2	TYR	H	94	35.653	15.907	2.642	1.00	3.12	H	C
ATOM	106	CZ	TYR	H	94	35.646	15.163	3.814	1.00	1.93	H	C
ATOM	107	OH	TYR	H	94	35.462	13.796	3.767	1.00	5.06	H	O
ATOM	108	N	VAL	H	95	39.254	17.656	3.584	1.00	8.23	H	N
ATOM	109	CA	VAL	H	95	39.989	16.748	2.713	1.00	8.13	H	C
ATOM	110	C	VAL	H	95	39.293	15.393	2.622	1.00	9.13	H	C
ATOM	111	O	VAL	H	95	39.141	14.692	3.625	1.00	8.17	H	O
ATOM	112	CB	VAL	H	95	41.428	16.523	3.225	1.00	8.63	H	C
ATOM	113	CG1	VAL	H	95	42.160	15.530	2.315	1.00	7.79	H	C
ATOM	114	CG2	VAL	H	95	42.173	17.848	3.271	1.00	9.62	H	C
ATOM	115	N	PRO	H	96	38.863	15.005	1.410	1.00	10.15	H	N
ATOM	116	CA	PRO	H	96	38.187	13.716	1.237	1.00	10.07	H	C
ATOM	117	C	PRO	H	96	38.988	12.623	1.928	1.00	9.71	H	C
ATOM	118	O	PRO	H	96	40.221	12.655	1.917	1.00	10.21	H	O
ATOM	119	CB	PRO	H	96	38.171	13.536	-0.279	1.00	9.81	H	C
ATOM	120	CG	PRO	H	96	38.070	14.949	-0.776	1.00	9.61	H	C
ATOM	121	CD	PRO	H	96	39.062	15.673	0.110	1.00	8.77	H	C
ATOM	122	N	GLY	H	97	38.280	11.675	2.534	1.00	7.35	H	N
ATOM	123	CA	GLY	H	97	38.928	10.571	3.222	1.00	7.72	H	C
ATOM	124	C	GLY	H	97	39.292	10.853	4.670	1.00	8.31	H	C
ATOM	125	O	GLY	H	97	39.656	9.934	5.404	1.00	5.90	H	O
ATOM	126	N	THR	H	98	39.187	12.112	5.091	1.00	8.38	H	N
ATOM	127	CA	THR	H	98	39.543	12.474	6.456	1.00	8.75	H	C
ATOM	128	C	THR	H	98	38.347	12.901	7.301	1.00	9.32	H	C
ATOM	129	O	THR	H	98	37.197	12.726	6.888	1.00	9.82	H	O
ATOM	130	CB	THR	H	98	40.639	13.572	6.474	1.00	10.03	H	C
ATOM	131	OG1	THR	H	98	40.118	14.798	5.939	1.00	9.30	H	O
ATOM	132	CG2	THR	H	98	41.841	13.123	5.636	1.00	7.92	H	C
ATOM	133	N	THR	H	99	38.622	13.478	8.470	1.00	6.94	H	N
ATOM	134	CA	THR	H	99	37.576	13.853	9.411	1.00	7.19	H	C
ATOM	135	C	THR	H	99	37.371	15.330	9.811	1.00	7.60	H	C
ATOM	136	O	THR	H	99	36.267	15.704	10.221	1.00	4.56	H	O
ATOM	137	CB	THR	H	99	37.761	13.028	10.697	1.00	9.01	H	C
ATOM	138	OG1	THR	H	99	39.126	13.133	11.128	1.00	8.28	H	O
ATOM	139	CG2	THR	H	99	37.434	11.556	10.444	1.00	8.22	H	C
ATOM	140	N	ASN	H	100	38.405	16.163	9.703	1.00	4.83	H	N
ATOM	141	CA	ASN	H	100	38.280	17.573	10.093	1.00	6.56	H	C
ATOM	142	C	ASN	H	100	37.359	18.369	9.157	1.00	6.18	H	C
ATOM	143	O	ASN	H	100	37.299	18.109	7.957	1.00	6.48	H	O
ATOM	144	CB	ASN	H	100	39.669	18.244	10.151	1.00	3.59	H	C
ATOM	145	CG	ASN	H	100	39.760	19.337	11.227	1.00	7.18	H	C
ATOM	146	OD1	ASN	H	100	40.685	20.162	11.222	1.00	9.38	H	O
ATOM	147	ND2	ASN	H	100	38.809	19.340	12.156	1.00	1.98	H	N
ATOM	148	N	HIS	H	101	36.638	19.338	9.718	1.00	6.06	H	N
ATOM	149	CA	HIS	H	101	35.725	20.178	8.940	1.00	6.01	H	C
ATOM	150	C	HIS	H	101	34.705	19.325	8.198	1.00	6.65	H	C
ATOM	151	O	HIS	H	101	34.433	19.562	7.017	1.00	6.05	H	O
ATOM	152	CB	HIS	H	101	36.510	21.018	7.927	1.00	6.13	H	C
ATOM	153	CG	HIS	H	101	37.589	21.853	8.541	1.00	9.14	H	C
ATOM	154	ND1	HIS	H	101	37.331	22.852	9.456	1.00	10.10	H	N
ATOM	155	CD2	HIS	H	101	38.935	21.824	8.387	1.00	8.84	H	C
ATOM	156	CE1	HIS	H	101	38.470	23.401	9.839	1.00	9.36	H	C
ATOM	157	NE2	HIS	H	101	39.458	22.795	9.206	1.00	5.86	H	N
ATOM	158	N	ASP	H	102	34.136	18.341	8.891	1.00	4.35	H	N
ATOM	159	CA	ASP	H	102	33.170	17.436	8.279	1.00	4.62	H	C
ATOM	160	C	ASP	H	102	31.773	18.055	8.310	1.00	5.36	H	C

ATOM	161	O	ASP	H	102	30.936	17.713	9.154	1.00	5.27	H O
ATOM	162	CB	ASP	H	102	33.188	16.095	9.016	1.00	1.00	H C
ATOM	163	CG	ASP	H	102	32.509	14.992	8.238	1.00	3.93	H C
ATOM	164	OD1	ASP	H	102	32.142	15.219	7.067	1.00	5.39	H O
ATOM	165	OD2	ASP	H	102	32.352	13.889	8.794	1.00	2.41	H O
ATOM	166	N	ILE	H	103	31.529	18.972	7.381	1.00	5.02	H N
ATOM	167	CA	ILE	H	103	30.248	19.659	7.309	1.00	3.77	H C
ATOM	168	C	ILE	H	103	29.945	20.059	5.874	1.00	4.55	H C
ATOM	169	O	ILE	H	103	30.851	20.349	5.094	1.00	4.54	H O
ATOM	170	CB	ILE	H	103	30.266	20.931	8.201	1.00	4.83	H C
ATOM	171	CG1	ILE	H	103	28.873	21.570	8.259	1.00	2.69	H C
ATOM	172	CG2	ILE	H	103	31.288	21.931	7.664	1.00	2.18	H C
ATOM	173	CD1	ILE	H	103	28.770	22.730	9.246	1.00	1.00	H C
ATOM	174	N	VAL	H	138	20.653	12.090	18.785	1.00	5.55	H N
ATOM	175	CA	VAL	H	138	21.298	11.812	17.509	1.00	6.30	H C
ATOM	176	C	VAL	H	138	20.336	10.842	16.823	1.00	6.56	H C
ATOM	177	O	VAL	H	138	19.741	9.990	17.479	1.00	7.54	H O
ATOM	178	CB	VAL	H	138	22.704	11.165	17.677	1.00	6.77	H C
ATOM	179	CG1	VAL	H	138	23.664	12.166	18.324	1.00	3.97	H C
ATOM	180	CG2	VAL	H	138	22.614	9.906	18.515	1.00	5.04	H C
ATOM	181	N	SER	H	139	20.172	10.967	15.512	1.00	6.69	H N
ATOM	182	CA	SER	H	139	19.227	10.114	14.805	1.00	5.72	H C
ATOM	183	C	SER	H	139	19.611	9.790	13.370	1.00	6.17	H C
ATOM	184	O	SER	H	139	20.485	10.431	12.787	1.00	5.98	H O
ATOM	185	CB	SER	H	139	17.850	10.786	14.815	1.00	6.76	H C
ATOM	186	OG	SER	H	139	17.944	12.120	14.327	1.00	4.59	H O
ATOM	187	N	GLY	H	142	20.741	4.754	9.987	1.00	8.09	H N
ATOM	188	CA	GLY	H	142	21.997	4.032	9.902	1.00	6.84	H C
ATOM	189	C	GLY	H	142	21.957	2.626	10.456	1.00	7.70	H C
ATOM	190	O	GLY	H	142	20.900	2.125	10.850	1.00	7.86	H O
ATOM	191	N	GLN	H	143	23.126	1.993	10.480	1.00	9.91	H N
ATOM	192	CA	GLN	H	143	23.278	0.628	10.976	1.00	11.50	H C
ATOM	193	C	GLN	H	143	22.843	0.499	12.425	1.00	11.62	H C
ATOM	194	O	GLN	H	143	23.133	1.360	13.255	1.00	10.73	H O
ATOM	195	CB	GLN	H	143	24.737	0.158	10.868	1.00	10.78	H C
ATOM	196	CG	GLN	H	143	25.309	0.056	9.452	1.00	13.60	H C
ATOM	197	CD	GLN	H	143	25.651	1.411	8.850	1.00	16.26	H C
ATOM	198	OE1	GLN	H	143	25.652	2.430	9.542	1.00	13.61	H O
ATOM	199	NE2	GLN	H	143	25.952	1.425	7.555	1.00	15.87	H N
ATOM	200	N	LEU	H	145	23.813	-2.024	14.132	1.00	17.85	H N
ATOM	201	CA	LEU	H	145	24.999	-2.630	14.718	1.00	21.26	H C
ATOM	202	C	LEU	H	145	26.174	-2.317	13.805	1.00	22.23	H C
ATOM	203	O	LEU	H	145	25.998	-2.080	12.610	1.00	20.28	H O
ATOM	204	CB	LEU	H	145	24.848	-4.149	14.816	1.00	21.41	H C
ATOM	205	CG	LEU	H	145	23.756	-4.748	15.699	1.00	24.05	H C
ATOM	206	CD1	LEU	H	145	23.709	-6.251	15.465	1.00	22.91	H C
ATOM	207	CD2	LEU	H	145	24.029	-4.437	17.166	1.00	24.83	H C
ATOM	208	N	ASP	H	146	27.371	-2.314	14.374	1.00	24.68	H N
ATOM	209	CA	ASP	H	146	28.569	-2.054	13.600	1.00	28.79	H C
ATOM	210	C	ASP	H	146	28.701	-3.221	12.634	1.00	30.65	H C
ATOM	211	O	ASP	H	146	28.649	-4.379	13.046	1.00	29.72	H O
ATOM	212	CB	ASP	H	146	29.781	-1.974	14.534	1.00	30.17	H C
ATOM	213	CG	ASP	H	146	31.076	-1.707	13.795	1.00	31.88	H C
ATOM	214	OD1	ASP	H	146	31.050	-0.995	12.767	1.00	32.57	H O
ATOM	215	OD2	ASP	H	146	32.128	-2.199	14.257	1.00	35.02	H O
ATOM	216	N	ARG	H	147	28.838	-2.918	11.348	1.00	34.10	H N

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ATOM    217  CA  ARG H 147      28.968  -3.964  10.338  1.00 37.74      H    C
ATOM    218  C   ARG H 147      27.620  -4.672  10.137  1.00 36.36      H    C
ATOM    219  O   ARG H 147      27.580  -5.856   9.805  1.00 38.70      H    O
ATOM    220  CB  ARG H 147      30.023  -4.977  10.794  1.00 41.63      H    C
ATOM    221  CG  ARG H 147      30.984  -5.462   9.731  1.00 48.94      H    C
ATOM    222  CD  ARG H 147      32.085  -6.279  10.395  1.00 55.34      H    C
ATOM    223  NE  ARG H 147      33.126  -6.706   9.465  1.00 60.79      H    N
ATOM    224  CZ  ARG H 147      34.228  -7.360   9.826  1.00 63.32      H    C
ATOM    225  NH1 ARG H 147      34.439  -7.667  11.100  1.00 64.90      H    N
ATOM    226  NH2 ARG H 147      35.122  -7.708   8.912  1.00 64.23      H    N
ATOM    227  N   LEU H 158      18.599   8.382  19.520  1.00  8.74      H    N
ATOM    228  CA  LEU H 158      19.340   8.024  20.727  1.00  7.23      H    C
ATOM    229  C   LEU H 158      19.751   9.261  21.527  1.00  8.93      H    C
ATOM    230  O   LEU H 158      20.116  10.290  20.953  1.00  8.07      H    O
ATOM    231  CB  LEU H 158      20.603   7.253  20.336  1.00  6.49      H    C
ATOM    232  CG  LEU H 158      21.572   6.875  21.454  1.00  6.44      H    C
ATOM    233  CD1 LEU H 158      20.931   5.804  22.334  1.00  7.20      H    C
ATOM    234  CD2 LEU H 158      22.886   6.374  20.853  1.00  6.24      H    C
ATOM    235  N   VAL H 160      22.440  10.884  23.870  1.00  6.69      H    N
ATOM    236  CA  VAL H 160      23.841  10.699  24.231  1.00  5.16      H    C
ATOM    237  C   VAL H 160      24.363  11.899  25.015  1.00  6.46      H    C
ATOM    238  O   VAL H 160      23.972  13.038  24.761  1.00  6.24      H    O
ATOM    239  CB  VAL H 160      24.748  10.493  22.977  1.00  4.79      H    C
ATOM    240  CG1 VAL H 160      24.364   9.202  22.248  1.00  2.87      H    C
ATOM    241  CG2 VAL H 160      24.636  11.690  22.033  1.00  4.14      H    C
ATOM    242  N   ARG H170C      40.277   4.649  25.092  1.00 26.96      H    N
ATOM    243  CA  ARG H170C      41.408   3.742  25.040  1.00 30.88      H    C
ATOM    244  C   ARG H170C      42.455   4.322  24.096  1.00 33.02      H    C
ATOM    245  O   ARG H170C      42.180   4.560  22.920  1.00 32.09      H    O
ATOM    246  CB  ARG H170C      40.952   2.368  24.546  1.00 32.33      H    C
ATOM    247  CG  ARG H170C      42.066   1.343  24.417  1.00 36.16      H    C
ATOM    248  CD  ARG H170C      41.510  -0.012  24.014  1.00 39.39      H    C
ATOM    249  NE  ARG H170C      42.563  -0.955  23.649  1.00 41.61      H    N
ATOM    250  CZ  ARG H170C      42.345  -2.177  23.169  1.00 44.13      H    C
ATOM    251  NH1 ARG H170C      41.105  -2.617  22.992  1.00 45.02      H    N
ATOM    252  NH2 ARG H170C      43.370  -2.959  22.859  1.00 45.11      H    N
ATOM    253  N   LYS H170D      43.650   4.565  24.622  1.00 36.30      H    N
ATOM    254  CA  LYS H170D      44.737   5.114  23.820  1.00 39.96      H    C
ATOM    255  C   LYS H170D      45.045   4.165  22.667  1.00 39.79      H    C
ATOM    256  O   LYS H170D      45.328   2.986  22.881  1.00 39.51      H    O
ATOM    257  CB  LYS H170D      45.986   5.302  24.685  1.00 43.00      H    C
ATOM    258  CG  LYS H170D      47.201   5.802  23.921  1.00 47.37      H    C
ATOM    259  CD  LYS H170D      48.433   5.842  24.812  1.00 51.67      H    C
ATOM    260  CE  LYS H170D      49.673   6.249  24.028  1.00 54.05      H    C
ATOM    261  NZ  LYS H170D      49.975   5.293  22.924  1.00 55.60      H    N
ATOM    262  N   VAL H170E      44.983   4.679  21.445  1.00 39.89      H    N
ATOM    263  CA  VAL H170E      45.250   3.860  20.269  1.00 40.30      H    C
ATOM    264  C   VAL H170E      46.447   4.372  19.472  1.00 41.06      H    C
ATOM    265  O   VAL H170E      47.128   5.312  19.888  1.00 41.71      H    O
ATOM    266  CB  VAL H170E      44.015   3.799  19.340  1.00 40.64      H    C
ATOM    267  CG1 VAL H170E      42.876   3.065  20.034  1.00 40.47      H    C
ATOM    268  CG2 VAL H170E      43.582   5.199  18.958  1.00 40.92      H    C
ATOM    269  N   GLY H170F      46.700   3.741  18.330  1.00 40.52      H    N
ATOM    270  CA  GLY H170F      47.814   4.140  17.492  1.00 39.24      H    C
ATOM    271  C   GLY H170F      47.649   5.534  16.920  1.00 38.47      H    C
ATOM    272  O   GLY H170F      47.270   6.468  17.630  1.00 38.87      H    O
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ATOM	273	N	ASP	H170G	47.932	5.672	15.629	1.00	36.20	H	N
ATOM	274	CA	ASP	H170G	47.823	6.955	14.951	1.00	34.41	H	C
ATOM	275	C	ASP	H170G	46.433	7.192	14.370	1.00	31.26	H	C
ATOM	276	O	ASP	H170G	46.265	7.306	13.155	1.00	30.19	H	O
ATOM	277	CB	ASP	H170G	48.869	7.049	13.839	1.00	38.35	H	C
ATOM	278	CG	ASP	H170G	50.282	7.112	14.377	1.00	42.44	H	C
ATOM	279	OD1	ASP	H170G	50.595	8.077	15.111	1.00	43.77	H	O
ATOM	280	OD2	ASP	H170G	51.080	6.200	14.069	1.00	44.37	H	O
ATOM	281	N	SER	H170H	45.438	7.265	15.245	1.00	27.38	H	N
ATOM	282	CA	SER	H170H	44.066	7.501	14.822	1.00	23.64	H	C
ATOM	283	C	SER	H170H	43.830	9.008	14.677	1.00	20.46	H	C
ATOM	284	O	SER	H170H	44.628	9.817	15.149	1.00	19.96	H	O
ATOM	285	CB	SER	H170H	43.096	6.902	15.846	1.00	24.30	H	C
ATOM	286	OG	SER	H170H	43.323	7.430	17.142	1.00	24.12	H	O
ATOM	287	N	PRO	H170I	42.733	9.403	14.013	1.00	17.84	H	N
ATOM	288	CA	PRO	H170I	42.432	10.826	13.826	1.00	15.01	H	C
ATOM	289	C	PRO	H170I	42.402	11.597	15.146	1.00	13.81	H	C
ATOM	290	O	PRO	H170I	41.933	11.090	16.162	1.00	11.82	H	O
ATOM	291	CB	PRO	H170I	41.066	10.798	13.142	1.00	14.13	H	C
ATOM	292	CG	PRO	H170I	41.112	9.519	12.359	1.00	15.60	H	C
ATOM	293	CD	PRO	H170I	41.716	8.562	13.358	1.00	16.03	H	C
ATOM	294	N	ASN	H 175	42.918	12.819	15.137	1.00	13.26	H	N
ATOM	295	CA	ASN	H 175	42.911	13.627	16.347	1.00	15.22	H	C
ATOM	296	C	ASN	H 175	41.540	14.261	16.497	1.00	12.70	H	C
ATOM	297	O	ASN	H 175	40.813	14.420	15.520	1.00	9.75	H	O
ATOM	298	CB	ASN	H 175	43.964	14.744	16.280	1.00	19.16	H	C
ATOM	299	CG	ASN	H 175	45.367	14.217	16.081	1.00	22.90	H	C
ATOM	300	OD1	ASN	H 175	45.726	13.159	16.597	1.00	28.38	H	O
ATOM	301	ND2	ASN	H 175	46.178	14.963	15.338	1.00	26.32	H	N
ATOM	302	N	ILE	H 176	41.190	14.609	17.729	1.00	12.09	H	N
ATOM	303	CA	ILE	H 176	39.922	15.270	18.015	1.00	10.80	H	C
ATOM	304	C	ILE	H 176	40.253	16.759	18.040	1.00	9.92	H	C
ATOM	305	O	ILE	H 176	40.856	17.248	18.992	1.00	8.78	H	O
ATOM	306	CB	ILE	H 176	39.373	14.856	19.391	1.00	10.52	H	C
ATOM	307	CG1	ILE	H 176	39.207	13.335	19.451	1.00	11.68	H	C
ATOM	308	CG2	ILE	H 176	38.032	15.533	19.636	1.00	7.09	H	C
ATOM	309	CD1	ILE	H 176	38.867	12.816	20.830	1.00	15.04	H	C
ATOM	310	N	MET	H 180	35.459	19.555	16.502	1.00	3.00	H	N
ATOM	311	CA	MET	H 180	34.757	18.321	16.843	1.00	3.79	H	C
ATOM	312	C	MET	H 180	34.487	18.263	18.344	1.00	4.77	H	C
ATOM	313	O	MET	H 180	35.007	19.075	19.114	1.00	6.30	H	O
ATOM	314	CB	MET	H 180	35.625	17.105	16.499	1.00	3.93	H	C
ATOM	315	CG	MET	H 180	36.365	17.162	15.169	1.00	5.58	H	C
ATOM	316	SD	MET	H 180	37.565	15.805	15.057	1.00	6.35	H	S
ATOM	317	CE	MET	H 180	38.175	16.035	13.399	1.00	4.33	H	C
ATOM	318	N	PHE	H 181	33.677	17.288	18.745	1.00	3.48	H	N
ATOM	319	CA	PHE	H 181	33.379	17.034	20.151	1.00	3.80	H	C
ATOM	320	C	PHE	H 181	32.851	15.608	20.242	1.00	4.05	H	C
ATOM	321	O	PHE	H 181	32.219	15.111	19.304	1.00	3.48	H	O
ATOM	322	CB	PHE	H 181	32.371	18.051	20.719	1.00	4.63	H	C
ATOM	323	CG	PHE	H 181	30.939	17.853	20.273	1.00	6.12	H	C
ATOM	324	CD1	PHE	H 181	30.134	16.881	20.863	1.00	3.60	H	C
ATOM	325	CD2	PHE	H 181	30.370	18.706	19.323	1.00	4.58	H	C
ATOM	326	CE1	PHE	H 181	28.777	16.767	20.519	1.00	4.70	H	C
ATOM	327	CE2	PHE	H 181	29.018	18.601	18.973	1.00	2.41	H	C
ATOM	328	CZ	PHE	H 181	28.220	17.634	19.572	1.00	4.06	H	C

ATOM	329	N	CYS	H	182	33.142	14.938	21.349	1.00	3.27	H	N
ATOM	330	CA	CYS	H	182	32.684	13.571	21.539	1.00	4.42	H	C
ATOM	331	C	CYS	H	182	31.373	13.550	22.298	1.00	3.93	H	C
ATOM	332	O	CYS	H	182	31.061	14.473	23.047	1.00	4.77	H	O
ATOM	333	CB	CYS	H	182	33.685	12.758	22.352	1.00	5.96	H	C
ATOM	334	SG	CYS	H	182	35.402	12.734	21.771	1.00	5.85	H	S
ATOM	335	N	ALA	H	183	30.619	12.476	22.112	1.00	3.91	H	N
ATOM	336	CA	ALA	H	183	29.356	12.290	22.810	1.00	5.23	H	C
ATOM	337	C	ALA	H	183	29.000	10.813	22.723	1.00	5.27	H	C
ATOM	338	O	ALA	H	183	29.318	10.150	21.740	1.00	7.26	H	O
ATOM	339	CB	ALA	H	183	28.254	13.152	22.178	1.00	2.74	H	C
ATOM	340	N	GLY	H	184A	28.361	10.289	23.760	1.00	7.33	H	N
ATOM	341	CA	GLY	H	184A	27.986	8.890	23.741	1.00	6.69	H	C
ATOM	342	C	GLY	H	184A	28.482	8.101	24.936	1.00	8.17	H	C
ATOM	343	O	GLY	H	184A	28.615	8.634	26.042	1.00	6.87	H	O
ATOM	344	N	TYR	H	184	28.771	6.825	24.699	1.00	7.70	H	N
ATOM	345	CA	TYR	H	184	29.224	5.921	25.750	1.00	8.19	H	C
ATOM	346	C	TYR	H	184	30.406	5.068	25.288	1.00	7.75	H	C
ATOM	347	O	TYR	H	184	30.506	4.712	24.114	1.00	6.46	H	O
ATOM	348	CB	TYR	H	184	28.074	5.004	26.176	1.00	8.95	H	C
ATOM	349	CG	TYR	H	184	26.813	5.725	26.615	1.00	10.41	H	C
ATOM	350	CD1	TYR	H	184	25.924	6.256	25.681	1.00	10.78	H	C
ATOM	351	CD2	TYR	H	184	26.515	5.881	27.967	1.00	10.54	H	C
ATOM	352	CE1	TYR	H	184	24.771	6.923	26.080	1.00	12.32	H	C
ATOM	353	CE2	TYR	H	184	25.369	6.542	28.378	1.00	12.03	H	C
ATOM	354	CZ	TYR	H	184	24.500	7.061	27.429	1.00	13.74	H	C
ATOM	355	OH	TYR	H	184	23.357	7.705	27.829	1.00	15.66	H	O
ATOM	356	N	LYS	H	188	25.832	2.110	23.136	1.00	8.03	H	N
ATOM	357	CA	LYS	H	188	25.079	3.077	22.349	1.00	7.40	H	C
ATOM	358	C	LYS	H	188	25.957	4.081	21.605	1.00	9.19	H	C
ATOM	359	O	LYS	H	188	26.946	4.585	22.147	1.00	7.00	H	O
ATOM	360	CB	LYS	H	188	24.123	3.820	23.283	1.00	8.96	H	C
ATOM	361	CG	LYS	H	188	23.123	2.911	24.006	1.00	9.81	H	C
ATOM	362	CD	LYS	H	188	22.325	3.672	25.051	1.00	11.33	H	C
ATOM	363	CE	LYS	H	188	23.157	3.965	26.292	1.00	14.58	H	C
ATOM	364	NZ	LYS	H	188	23.504	2.721	27.048	1.00	14.57	H	N
ATOM	365	N	ASP	H	189	25.570	4.397	20.373	1.00	6.80	H	N
ATOM	366	CA	ASP	H	189	26.350	5.319	19.560	1.00	8.44	H	C
ATOM	367	C	ASP	H	189	25.650	5.465	18.209	1.00	8.51	H	C
ATOM	368	O	ASP	H	189	24.752	4.686	17.886	1.00	7.47	H	O
ATOM	369	CB	ASP	H	189	27.755	4.705	19.393	1.00	9.61	H	C
ATOM	370	CG	ASP	H	189	28.738	5.610	18.677	1.00	8.64	H	C
ATOM	371	OD1	ASP	H	189	28.457	6.811	18.489	1.00	9.82	H	O
ATOM	372	OD2	ASP	H	189	29.819	5.098	18.313	1.00	6.31	H	O
ATOM	373	N	SER	H	190	26.013	6.486	17.441	1.00	6.24	H	N
ATOM	374	CA	SER	H	190	25.450	6.628	16.106	1.00	6.22	H	C
ATOM	375	C	SER	H	190	26.395	5.773	15.249	1.00	7.07	H	C
ATOM	376	O	SER	H	190	27.367	5.221	15.775	1.00	5.91	H	O
ATOM	377	CB	SER	H	190	25.450	8.101	15.658	1.00	4.21	H	C
ATOM	378	OG	SER	H	190	26.703	8.733	15.861	1.00	4.59	H	O
ATOM	379	N	CYS	H	191	26.128	5.641	13.953	1.00	8.36	H	N
ATOM	380	CA	CYS	H	191	26.992	4.823	13.099	1.00	7.99	H	C
ATOM	381	C	CYS	H	191	27.131	5.428	11.698	1.00	8.96	H	C
ATOM	382	O	CYS	H	191	26.507	6.442	11.388	1.00	8.95	H	O
ATOM	383	CB	CYS	H	191	26.446	3.384	13.036	1.00	8.01	H	C
ATOM	384	SG	CYS	H	191	27.624	2.081	12.512	1.00	11.48	H	S

ATOM	385	N	LYS	H	192	27.955	4.804	10.861	1.00	9.23	H N
ATOM	386	CA	LYS	H	192	28.232	5.291	9.508	1.00	10.49	H C
ATOM	387	C	LYS	H	192	27.042	5.787	8.691	1.00	9.74	H C
ATOM	388	O	LYS	H	192	27.089	6.885	8.131	1.00	9.42	H O
ATOM	389	CB	LYS	H	192	28.996	4.221	8.720	1.00	12.99	H C
ATOM	390	CG	LYS	H	192	30.288	3.788	9.406	1.00	17.47	H C
ATOM	391	CD	LYS	H	192	31.180	2.948	8.509	1.00	21.20	H C
ATOM	392	CE	LYS	H	192	32.448	2.535	9.258	1.00	25.68	H C
ATOM	393	NZ	LYS	H	192	33.427	1.809	8.395	1.00	28.01	H N
ATOM	394	N	GLY	H	193	25.983	4.989	8.623	1.00	9.29	H N
ATOM	395	CA	GLY	H	193	24.806	5.380	7.863	1.00	9.11	H C
ATOM	396	C	GLY	H	193	24.059	6.573	8.433	1.00	10.62	H C
ATOM	397	O	GLY	H	193	23.188	7.141	7.774	1.00	12.70	H O
ATOM	398	N	ASP	H	194	24.386	6.959	9.662	1.00	8.84	H N
ATOM	399	CA	ASP	H	194	23.744	8.108	10.289	1.00	7.33	H C
ATOM	400	C	ASP	H	194	24.475	9.412	9.972	1.00	7.03	H C
ATOM	401	O	ASP	H	194	23.989	10.492	10.312	1.00	7.04	H O
ATOM	402	CB	ASP	H	194	23.688	7.917	11.802	1.00	5.37	H C
ATOM	403	CG	ASP	H	194	22.927	6.671	12.195	1.00	7.85	H C
ATOM	404	OD1	ASP	H	194	21.737	6.572	11.833	1.00	6.73	H O
ATOM	405	OD2	ASP	H	194	23.519	5.794	12.857	1.00	4.09	H O
ATOM	406	N	SER	H	195	25.634	9.301	9.324	1.00	5.05	H N
ATOM	407	CA	SER	H	195	26.449	10.454	8.960	1.00	5.57	H C
ATOM	408	C	SER	H	195	25.629	11.601	8.387	1.00	6.98	H C
ATOM	409	O	SER	H	195	24.730	11.391	7.573	1.00	4.66	H O
ATOM	410	CB	SER	H	195	27.521	10.050	7.939	1.00	4.83	H C
ATOM	411	OG	SER	H	195	28.461	9.156	8.509	1.00	2.83	H O
ATOM	412	N	GLY	H	196	25.958	12.817	8.816	1.00	7.56	H N
ATOM	413	CA	GLY	H	196	25.253	13.994	8.337	1.00	7.44	H C
ATOM	414	C	GLY	H	196	24.032	14.324	9.174	1.00	7.23	H C
ATOM	415	O	GLY	H	196	23.564	15.460	9.178	1.00	7.34	H O
ATOM	416	N	GLY	H	197	23.520	13.325	9.888	1.00	7.25	H N
ATOM	417	CA	GLY	H	197	22.351	13.517	10.721	1.00	5.90	H C
ATOM	418	C	GLY	H	197	22.572	14.494	11.858	1.00	6.34	H C
ATOM	419	O	GLY	H	197	23.707	14.824	12.195	1.00	7.23	H O
ATOM	420	N	HIS	H	199	22.592	16.228	15.752	1.00	4.66	H N
ATOM	421	CA	HIS	H	199	22.920	16.007	17.151	1.00	2.68	H C
ATOM	422	C	HIS	H	199	22.168	17.243	17.628	1.00	3.98	H C
ATOM	423	O	HIS	H	199	22.668	18.366	17.497	1.00	4.27	H O
ATOM	424	CB	HIS	H	199	24.424	16.155	17.391	1.00	4.75	H C
ATOM	425	CG	HIS	H	199	24.812	16.159	18.838	1.00	3.77	H C
ATOM	426	ND1	HIS	H	199	24.693	17.275	19.636	1.00	1.00	H N
ATOM	427	CD2	HIS	H	199	25.308	15.179	19.633	1.00	4.02	H C
ATOM	428	CE1	HIS	H	199	25.103	16.987	20.858	1.00	2.26	H C
ATOM	429	NE2	HIS	H	199	25.481	15.721	20.883	1.00	2.92	H N
ATOM	430	N	ILE	H	212	26.974	17.242	14.214	1.00	5.45	H N
ATOM	431	CA	ILE	H	212	26.692	16.454	13.021	1.00	5.68	H C
ATOM	432	C	ILE	H	212	27.372	15.092	13.160	1.00	6.39	H C
ATOM	433	O	ILE	H	212	28.561	15.029	13.458	1.00	7.22	H O
ATOM	434	CB	ILE	H	212	27.265	17.133	11.753	1.00	5.98	H C
ATOM	435	CG1	ILE	H	212	26.699	18.545	11.606	1.00	4.14	H C
ATOM	436	CG2	ILE	H	212	26.943	16.296	10.522	1.00	5.31	H C
ATOM	437	CD1	ILE	H	212	27.426	19.368	10.561	1.00	3.83	H C
ATOM	438	N	VAL	H	213	26.620	14.010	12.962	1.00	6.29	H N
ATOM	439	CA	VAL	H	213	27.187	12.661	13.039	1.00	3.02	H C
ATOM	440	C	VAL	H	213	28.340	12.692	12.046	1.00	3.61	H C

ATOM	441	O	VAL	H	213	28.130	12.905	10.846	1.00	3.84	H	O
ATOM	442	CB	VAL	H	213	26.149	11.581	12.617	1.00	1.61	H	C
ATOM	443	CG1	VAL	H	213	26.792	10.194	12.636	1.00	1.00	H	C
ATOM	444	CG2	VAL	H	213	24.959	11.599	13.578	1.00	1.00	H	C
ATOM	445	N	SER	H	214	29.557	12.491	12.540	1.00	4.04	H	N
ATOM	446	CA	SER	H	214	30.728	12.582	11.675	1.00	5.26	H	C
ATOM	447	C	SER	H	214	31.619	11.349	11.577	1.00	3.67	H	C
ATOM	448	O	SER	H	214	31.766	10.778	10.497	1.00	3.00	H	O
ATOM	449	CB	SER	H	214	31.561	13.794	12.101	1.00	4.06	H	C
ATOM	450	OG	SER	H	214	32.746	13.898	11.343	1.00	7.47	H	O
ATOM	451	N	TRP	H	215	32.225	10.946	12.689	1.00	2.06	H	N
ATOM	452	CA	TRP	H	215	33.094	9.779	12.667	1.00	4.11	H	C
ATOM	453	C	TRP	H	215	33.247	9.099	14.018	1.00	5.89	H	C
ATOM	454	O	TRP	H	215	32.628	9.491	15.007	1.00	5.44	H	O
ATOM	455	CB	TRP	H	215	34.489	10.148	12.120	1.00	5.71	H	C
ATOM	456	CG	TRP	H	215	35.298	11.099	12.983	1.00	6.60	H	C
ATOM	457	CD1	TRP	H	215	35.174	12.459	13.046	1.00	8.26	H	C
ATOM	458	CD2	TRP	H	215	36.374	10.755	13.870	1.00	7.17	H	C
ATOM	459	NE1	TRP	H	215	36.106	12.985	13.910	1.00	6.83	H	N
ATOM	460	CE2	TRP	H	215	36.855	11.962	14.433	1.00	7.22	H	C
ATOM	461	CE3	TRP	H	215	36.979	9.546	14.244	1.00	6.60	H	C
ATOM	462	CZ2	TRP	H	215	37.912	11.996	15.351	1.00	4.55	H	C
ATOM	463	CZ3	TRP	H	215	38.035	9.578	15.161	1.00	7.36	H	C
ATOM	464	CH2	TRP	H	215	38.488	10.799	15.703	1.00	6.87	H	C
ATOM	465	N	GLY	H	216	34.086	8.070	14.043	1.00	6.33	H	N
ATOM	466	CA	GLY	H	216	34.336	7.332	15.265	1.00	8.66	H	C
ATOM	467	C	GLY	H	216	35.004	6.017	14.932	1.00	9.66	H	C
ATOM	468	O	GLY	H	216	34.914	5.543	13.795	1.00	9.71	H	O
ATOM	469	N	GLN	H	217	35.684	5.422	15.906	1.00	10.43	H	N
ATOM	470	CA	GLN	H	217	36.346	4.148	15.669	1.00	10.60	H	C
ATOM	471	C	GLN	H	217	35.284	3.065	15.765	1.00	10.61	H	C
ATOM	472	O	GLN	H	217	34.858	2.695	16.858	1.00	13.71	H	O
ATOM	473	CB	GLN	H	217	37.449	3.919	16.701	1.00	12.43	H	C
ATOM	474	CG	GLN	H	217	38.205	2.612	16.498	1.00	14.99	H	C
ATOM	475	CD	GLN	H	217	39.564	2.605	17.171	1.00	18.06	H	C
ATOM	476	OE1	GLN	H	217	40.134	1.540	17.427	1.00	19.54	H	O
ATOM	477	NE2	GLN	H	217	40.103	3.794	17.443	1.00	13.50	H	N
ATOM	478	N	GLY	H	219	34.854	2.563	14.612	1.00	10.68	H	N
ATOM	479	CA	GLY	H	219	33.803	1.563	14.596	1.00	11.37	H	C
ATOM	480	C	GLY	H	219	32.536	2.218	15.126	1.00	11.52	H	C
ATOM	481	O	GLY	H	219	32.436	3.446	15.163	1.00	11.41	H	O
ATOM	482	N	CYS	H	220	31.569	1.410	15.542	1.00	11.97	H	N
ATOM	483	CA	CYS	H	220	30.317	1.934	16.077	1.00	11.90	H	C
ATOM	484	C	CYS	H	220	30.052	1.266	17.420	1.00	11.82	H	C
ATOM	485	O	CYS	H	220	29.975	0.037	17.508	1.00	12.68	H	O
ATOM	486	CB	CYS	H	220	29.170	1.658	15.099	1.00	11.56	H	C
ATOM	487	SG	CYS	H	220	29.346	2.521	13.505	1.00	8.67	H	S
ATOM	488	N	ALA	H	221A	29.916	2.084	18.462	1.00	10.74	H	N
ATOM	489	CA	ALA	H	221A	29.691	1.588	19.817	1.00	10.47	H	C
ATOM	490	C	ALA	H	221A	30.806	0.616	20.198	1.00	10.93	H	C
ATOM	491	O	ALA	H	221A	30.547	-0.493	20.677	1.00	11.08	H	O
ATOM	492	CB	ALA	H	221A	28.336	0.901	19.914	1.00	11.15	H	C
ATOM	493	N	THR	H	221	32.046	1.045	19.968	1.00	9.44	H	N
ATOM	494	CA	THR	H	221	33.237	0.249	20.274	1.00	8.66	H	C
ATOM	495	C	THR	H	221	33.708	0.543	21.695	1.00	8.04	H	C
ATOM	496	O	THR	H	221	33.859	1.706	22.075	1.00	7.03	H	O

ATOM	497	CB	THR	H	221	34.391	0.578	19.289	1.00	8.20	H C
ATOM	498	OG1	THR	H	221	33.983	0.265	17.951	1.00	10.25	H O
ATOM	499	CG2	THR	H	221	35.634	-0.225	19.623	1.00	11.22	H C
ATOM	500	N	VAL	H	222	33.926	-0.508	22.480	1.00	7.75	H N
ATOM	501	CA	VAL	H	222	34.386	-0.361	23.862	1.00	7.14	H C
ATOM	502	C	VAL	H	222	35.637	0.508	23.904	1.00	7.56	H C
ATOM	503	O	VAL	H	222	36.567	0.304	23.132	1.00	7.65	H O
ATOM	504	CB	VAL	H	222	34.705	-1.745	24.507	1.00	6.51	H C
ATOM	505	CG1	VAL	H	222	35.329	-1.558	25.893	1.00	6.03	H C
ATOM	506	CG2	VAL	H	222	33.426	-2.564	24.629	1.00	4.73	H C
ATOM	507	N	HIS	H	224	35.632	3.718	23.234	1.00	6.63	H N
ATOM	508	CA	HIS	H	224	35.512	4.808	22.269	1.00	7.22	H C
ATOM	509	C	HIS	H	224	34.148	5.500	22.271	1.00	7.59	H C
ATOM	510	O	HIS	H	224	33.127	4.906	22.618	1.00	8.49	H O
ATOM	511	CB	HIS	H	224	35.840	4.300	20.862	1.00	8.31	H C
ATOM	512	CG	HIS	H	224	37.279	3.936	20.682	1.00	10.98	H C
ATOM	513	ND1	HIS	H	224	38.276	4.881	20.572	1.00	10.97	H N
ATOM	514	CD2	HIS	H	224	37.899	2.731	20.668	1.00	12.41	H C
ATOM	515	CE1	HIS	H	224	39.448	4.277	20.501	1.00	11.73	H C
ATOM	516	NE2	HIS	H	224	39.247	2.973	20.557	1.00	14.76	H N
ATOM	517	N	PHE	H	225	34.157	6.770	21.881	1.00	7.18	H N
ATOM	518	CA	PHE	H	225	32.960	7.596	21.822	1.00	6.04	H C
ATOM	519	C	PHE	H	225	32.725	8.038	20.381	1.00	7.09	H C
ATOM	520	O	PHE	H	225	33.657	8.075	19.573	1.00	9.02	H O
ATOM	521	CB	PHE	H	225	33.151	8.870	22.659	1.00	5.47	H C
ATOM	522	CG	PHE	H	225	33.293	8.634	24.136	1.00	6.44	H C
ATOM	523	CD1	PHE	H	225	32.171	8.572	24.954	1.00	2.41	H C
ATOM	524	CD2	PHE	H	225	34.554	8.511	24.716	1.00	4.55	H C
ATOM	525	CE1	PHE	H	225	32.303	8.397	26.333	1.00	5.42	H C
ATOM	526	CE2	PHE	H	225	34.694	8.335	26.089	1.00	5.19	H C
ATOM	527	CZ	PHE	H	225	33.565	8.280	26.900	1.00	3.44	H C
ATOM	528	N	GLY	H	226	31.485	8.392	20.065	1.00	5.55	H N
ATOM	529	CA	GLY	H	226	31.197	8.893	18.734	1.00	5.48	H C
ATOM	530	C	GLY	H	226	31.753	10.313	18.667	1.00	5.81	H C
ATOM	531	O	GLY	H	226	31.837	10.990	19.695	1.00	4.00	H O
ATOM	532	N	VAL	H	227	32.151	10.760	17.479	1.00	3.76	H N
ATOM	533	CA	VAL	H	227	32.693	12.107	17.312	1.00	5.52	H C
ATOM	534	C	VAL	H	227	31.800	12.883	16.347	1.00	5.53	H C
ATOM	535	O	VAL	H	227	31.436	12.389	15.277	1.00	3.89	H O
ATOM	536	CB	VAL	H	227	34.142	12.088	16.764	1.00	5.30	H C
ATOM	537	CG1	VAL	H	227	34.725	13.500	16.812	1.00	3.32	H C
ATOM	538	CG2	VAL	H	227	35.000	11.126	17.576	1.00	1.00	H C
ATOM	539	N	TYR	H	228	31.467	14.108	16.734	1.00	5.76	H N
ATOM	540	CA	TYR	H	228	30.566	14.947	15.959	1.00	5.23	H C
ATOM	541	C	TYR	H	228	31.190	16.277	15.556	1.00	4.97	H C
ATOM	542	O	TYR	H	228	32.007	16.833	16.282	1.00	4.90	H O
ATOM	543	CB	TYR	H	228	29.291	15.203	16.781	1.00	6.48	H C
ATOM	544	CG	TYR	H	228	28.564	13.935	17.216	1.00	7.32	H C
ATOM	545	CD1	TYR	H	228	29.046	13.138	18.264	1.00	8.15	H C
ATOM	546	CD2	TYR	H	228	27.432	13.500	16.531	1.00	6.35	H C
ATOM	547	CE1	TYR	H	228	28.408	11.929	18.603	1.00	9.05	H C
ATOM	548	CE2	TYR	H	228	26.801	12.316	16.857	1.00	7.95	H C
ATOM	549	CZ	TYR	H	228	27.287	11.532	17.885	1.00	8.70	H C
ATOM	550	OH	TYR	H	228	26.647	10.347	18.158	1.00	8.64	H O
ATOM	551	N	THR	H	229	30.807	16.784	14.389	1.00	4.04	H N
ATOM	552	CA	THR	H	229	31.329	18.067	13.929	1.00	4.70	H C

ATOM	553	C	THR	H	229	30.782	19.121	14.900	1.00	3.38	H	C
ATOM	554	O	THR	H	229	29.590	19.133	15.181	1.00	3.30	H	O
ATOM	555	CB	THR	H	229	30.836	18.381	12.504	1.00	5.34	H	C
ATOM	556	OG1	THR	H	229	31.188	17.301	11.627	1.00	6.83	H	O
ATOM	557	CG2	THR	H	229	31.461	19.668	11.998	1.00	2.01	H	C
ATOM	558	C11	142	I	1	35.781	7.018	10.285	1.00	12.37	I	C
ATOM	559	O2	142	I	1	34.889	7.239	11.100	1.00	10.13	I	O
ATOM	560	N4	142	I	1	35.803	7.455	9.001	1.00	10.92	I	N
ATOM	561	C10	142	I	1	34.710	8.250	8.481	1.00	9.56	I	C
ATOM	562	C13	142	I	1	34.848	8.535	6.994	1.00	8.40	I	C
ATOM	563	C14	142	I	1	36.165	9.222	6.602	1.00	6.40	I	C
ATOM	564	C9	142	I	1	33.397	7.494	8.773	1.00	10.00	I	C
ATOM	565	O1	142	I	1	33.289	6.279	8.607	1.00	8.42	I	O
ATOM	566	N3	142	I	1	32.427	8.295	9.230	1.00	8.14	I	N
ATOM	567	C8	142	I	1	31.166	7.668	9.494	1.00	7.12	I	C
ATOM	568	C6	142	I	1	31.799	6.529	11.670	1.00	3.93	I	C
ATOM	569	C7	142	I	1	31.539	6.286	13.035	1.00	6.62	I	C
ATOM	570	C2	142	I	1	30.475	6.947	13.697	1.00	4.23	I	C
ATOM	571	C3	142	I	1	29.626	7.773	12.954	1.00	3.55	I	C
ATOM	572	C4	142	I	1	29.868	7.994	11.603	1.00	5.96	I	C
ATOM	573	C5	142	I	1	30.952	7.384	10.951	1.00	6.87	I	C
ATOM	574	C1	142	I	1	30.247	6.782	15.131	1.00	4.86	I	C
ATOM	575	N1	142	I	1	30.808	5.783	15.789	1.00	2.27	I	N
ATOM	576	C15	142	I	1	36.036	9.591	5.142	1.00	7.71	I	C
ATOM	577	O5	142	I	1	35.840	8.729	4.291	1.00	11.38	I	O
ATOM	578	N6	142	I	1	36.066	10.898	4.897	1.00	6.65	I	N
ATOM	579	C16	142	I	1	37.992	7.122	11.404	1.00	12.61	I	C
ATOM	580	N5	142	I	1	36.563	5.104	11.541	1.00	16.04	I	N
ATOM	581	C12	142	I	1	37.009	6.187	10.696	1.00	13.72	I	C
ATOM	582	S1	142	I	1	36.372	3.520	10.904	1.00	19.57	I	S
ATOM	583	O4	142	I	1	35.680	3.703	9.668	1.00	20.77	I	O
ATOM	584	O3	142	I	1	35.734	2.849	11.987	1.00	18.06	I	O
ATOM	585	C29	142	I	1	37.958	2.804	10.578	1.00	19.56	I	C
ATOM	586	C30	142	I	1	38.640	3.369	9.320	1.00	26.52	I	C
ATOM	587	N2	142	I	1	29.435	7.589	15.802	1.00	2.52	I	N
ATOM	588	C22	142	I	1	40.253	6.007	11.120	1.00	13.78	I	C
ATOM	589	C17	142	I	1	39.172	6.378	11.945	1.00	12.60	I	C
ATOM	590	C18	142	I	1	39.260	5.996	13.297	1.00	13.94	I	C
ATOM	591	C19	142	I	1	40.362	5.257	13.785	1.00	14.86	I	C
ATOM	592	C20	142	I	1	41.430	4.868	12.954	1.00	14.31	I	C
ATOM	593	C21	142	I	1	41.350	5.273	11.615	1.00	12.85	I	C
ATOM	594	C27	142	I	1	45.001	3.681	13.710	1.00	18.09	I	C
ATOM	595	C28	142	I	1	43.904	4.357	13.114	1.00	16.71	I	C
ATOM	596	C23	142	I	1	42.573	4.077	13.477	1.00	15.00	I	C
ATOM	597	C24	142	I	1	42.385	3.038	14.411	1.00	17.61	I	C
ATOM	598	C25	142	I	1	43.473	2.352	15.002	1.00	18.20	I	C
ATOM	599	C26	142	I	1	44.803	2.684	14.686	1.00	18.30	I	C
ATOM	600	OH2	WAT	W	2	21.173	10.598	10.229	1.00	2.46	W	O
ATOM	601	OH2	WAT	W	3	41.236	15.367	9.038	1.00	9.89	W	O
ATOM	602	OH2	WAT	W	11	39.351	17.218	6.324	1.00	2.98	W	O
ATOM	603	OH2	WAT	W	16	28.951	6.415	21.747	1.00	8.07	W	O
ATOM	604	OH2	WAT	W	17	36.844	8.297	21.377	1.00	8.16	W	O
ATOM	605	OH2	WAT	W	19	29.393	7.360	5.894	1.00	10.69	W	O
ATOM	606	OH2	WAT	W	22	40.618	0.517	20.963	1.00	12.88	W	O
ATOM	607	OH2	WAT	W	41	20.474	8.594	8.383	1.00	2.92	W	O
ATOM	608	OH2	WAT	W	43	33.354	15.140	0.160	1.00	4.35	W	O

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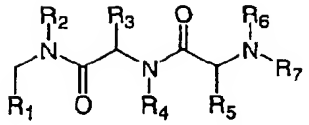
ATOM    609  OH2 WAT W  52      41.064  11.721   9.444  1.00 11.25      W    O
ATOM    610  OH2 WAT W  55      31.078   4.628  20.839  1.00 19.21      W    O
ATOM    611  OH2 WAT W  73      31.424   2.387  23.087  1.00 16.83      W    O
ATOM    612  OH2 WAT W  90      34.297  16.904  -1.657  1.00  8.85      W    O
ATOM    613  OH2 WAT W  92      34.705  15.756  12.306  1.00  4.39      W    O
ATOM    614  OH2 WAT W  97      32.609   3.792  18.618  1.00 10.06      W    O
ATOM    615  OH2 WAT W 113      29.869   9.653  -1.073  1.00 13.89      W    O
ATOM    616  OH2 WAT W 115      27.599   8.830  20.107  1.00  6.50      W    O
ATOM    617  OH2 WAT W 119      35.741   6.643  18.640  1.00 13.65      W    O
ATOM    618  OH2 WAT W 132      38.202   7.871  19.316  1.00 21.67      W    O
ATOM    619  OH2 WAT W 133      39.823   6.712  17.466  1.00 16.74      W    O
ATOM    620  OH2 WAT W 167      45.149   0.561  24.578  1.00 31.52      W    O
ATOM    621  OH2 WAT W 169      26.773   3.657   5.750  1.00 20.71      W    O
ATOM    622  OH2 WAT W 179      33.910  15.111  -3.886  1.00 26.31      W    O
ATOM    623  OH2 WAT W 183      22.630   6.394   5.218  1.00 17.19      W    O
ATOM    624  OH2 WAT W 190      41.408   8.993  17.609  1.00 38.16      W    O
ATOM    625  OH2 WAT W 208      28.879   7.652  -2.728  1.00 25.34      W    O
ATOM    626  OH2 WAT W 211      40.187   8.447  20.906  1.00 29.06      W    O
ATOM    627  OH2 WAT W 223      41.040  14.573  12.781  1.00 21.90      W    O
ATOM    628  OH2 WAT W 279      28.609  -2.348  19.633  1.00 16.06      W    O
ATOM    629  OH2 WAT W 287      27.925  -2.786  17.100  1.00 28.20      W    O
ATOM    630  OH2 WAT W 292      29.248  10.608  15.460  1.00  4.55      W    O
ATOM    631  OH2 WAT W 294      34.711  11.933   8.259  1.00 18.60      W    O
ATOM    632  OH2 WAT W 296      36.499   8.641   1.251  1.00 16.68      W    O
ATOM    633  OH2 WAT W 302      33.346   8.640   3.104  1.00 31.25      W    O
ATOM    634  OH2 WAT W 314      38.929  -1.342  19.839  1.00 27.36      W    O
ATOM    635  OH2 WAT W 319      24.988   4.849   4.100  1.00 39.67      W    O
ATOM    636  OH2 WAT W 321      38.601  -1.114  16.775  1.00 24.51      W    O
ATOM    637  OH2 WAT W 327      39.896   8.788   8.314  1.00 40.66      W    O
ATOM    638  OH2 WAT W 335      44.187  13.742  12.663  1.00 29.57      W    O
ATOM    639  OH2 WAT W 337      27.275   6.739   2.616  1.00 23.30      W    O
ATOM    640  OH2 WAT W 343      34.463   4.647   6.797  1.00 34.65      W    O
ATOM    641  OH2 WAT W 358      35.750  -0.120   8.819  1.00 35.63      W    O
ATOM    642  OH2 WAT W 370      38.235   6.328   7.390  1.00 28.92      W    O
ATOM    643  OH2 WAT W 388      42.864   7.185   8.805  1.00 39.53      W    O
ATOM    644  OH2 WAT W 390      31.573   8.191   0.869  1.00 38.78      W    O
ATOM    645  OH2 WAT W 401      41.353   4.533   8.074  1.00 36.07      W    O
ATOM    646  OH2 WAT W 402      29.643  -0.022  10.304  1.00 38.02      W    O
ATOM    647  OH2 WAT W 433      44.330   8.280  11.373  1.00 43.93      W    O
ATOM    648  OH2 WAT W 440      29.301  -0.100   7.598  1.00 43.24      W    O
ATOM    649  OH2 WAT W 446      38.570   9.454  -0.831  1.00 41.14      W    O
ATOM    650  OH2 WAT W 447      42.864  11.302   1.981  1.00 29.17      W    O
ATOM    651  OH2 WAT W 448      44.322  12.556   8.806  1.00 50.64      W    O
ATOM    652  OH2 WAT W 452      41.748  10.947  19.697  1.00 41.61      W    O
ATOM    653  OH2 WAT W 454      38.170   6.670   2.158  1.00 38.30      W    O
END
```

Claims

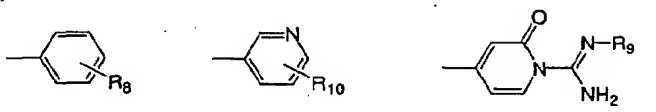
1. A compound of Formula (1):

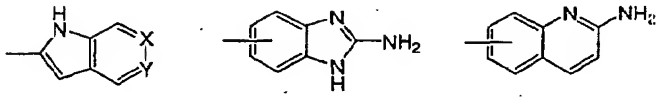


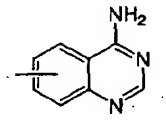
(1)

wherein

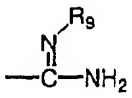
R_1 represents a group selected from the following formulae:







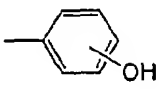
[wherein R_8 represents an amino group, an aminomethyl group or



(wherein R_9 represents a hydrogen atom, an amino group, a hydroxy group, an acyl group or an alkoxycarbonyl group having an optionally substituted linear or branched C_1-C_6 alkyl as its alkyl moiety, R_{10} represents an amino group, one of X and Y represents =CH- and the other represents =N-)];

R_2 represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group;

R_3 represents:

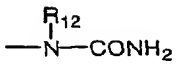


or

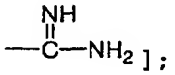
$$-(CH_2)_m-R_{11}$$

[wherein m represents an integer of 1 to 6, and R_{11} represents:

$-CONH_2$,



(wherein R_{12} represents a hydrogen atom or a linear or branched C_1-C_3 alkyl group) or



R_4 represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group;

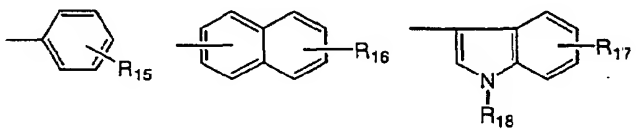
R_5 represents a linear or branched C_1-C_6 alkyl group or $-CH_2-R_{13}$ (wherein R_{13} represents an optionally substituted aryl group or an optionally substituted heterocyclic group);

R_6 represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group; and

R_7 represents an optionally substituted linear or branched C_1-C_6 alkyl group or $-SO_2-R_{14}$ (wherein R_{14} represents an optionally substituted linear or branched C_1-C_8 alkyl group)

or a tautomer or enantiomer of the compound, or a hydrate or pharmaceutically acceptable salt thereof.

2. The compound according to claim 1, wherein. R_5 in Formula (1) is a linear or branched C_1-C_6 alkyl group or-CH_2-R_{13}, in which R_{13} represents a group selected from the following formulae:

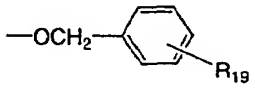


[wherein

R_{15} represents a hydrogen atom, an optionally substituted aryl group, a C_1-C_3 alkyl group which may be substituted with a halogen atom, a linear or branched C_1-C_3 alkoxy group, a halogen atom, an arylcarbonyl group, an alkylcarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety, a nitro group, or an amino group;

R_{16} represents a hydrogen atom or a linear or branched C_1-C_6 alkyl group;

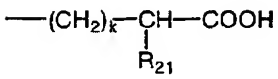
R_{17} represents a hydrogen atom, a hydroxy group, a linear or branched C_1-C_6 alkyl group, a linear or branched C_1-C_6 alkoxy group, $-O-(CH_2)_n-OH$ (wherein n represents an integer of 1 to 5), $-O-(CH_2)_p-COOH$ (wherein p represents an integer of 1 to 5), $-O-(CH_2)_q-NH_2$ (wherein q represents an integer of 1 to 5),



(wherein R_{19} represents a hydrogen atom, a hydroxy group, a carboxyl group, a linear or branched C_1-C_6 alkyl group, a halogen atom, a linear or branched C_1-C_6 alkoxy group, or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety), or $-OSO_2-R_{20}$ (wherein R_{20} represents a linear or branched C_1-C_6 alkyl group or a benzyl group); and

R_{18} represents a hydrogen atom, a linear or branched C_1-C_6 alkyl group, a linear or branched C_1-C_6 alkylsulfonyl group, or an optionally substituted arylsulfonyl group].

3. The compound according to claim 1 or 2, wherein R_7 in Formula (1) is a linear or branched C_1-C_6 alkyl group or a group of the following formula:



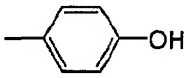
[wherein k represents an integer of 0 to 3, and R_{21} represents a hydrogen atom or -NHR_{22} (wherein R_{22} represents a linear or branched C_1-C_3 alkyl group or an alkylcarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety)] or

$$-SO_2-R_{14}$$

[wherein R_{14} represents:

(i) an optionally substituted linear or branched C_1-C_6 alkyl group (wherein said alkyl group may be substituted with a carboxyl group or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety); or
(ii) -CH_2-R_{23} (wherein R_{23} represents an optionally substituted phenyl group)].

4. The compound according to any one of claims 1 to 3, wherein R_3 in Formula (1) is a group of the following formula:

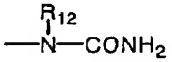


or

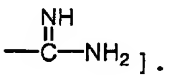
$$-(CH_2)_m-R_{11}$$

[wherein m represents an integer of 1 to 3, and R_{11} represents:

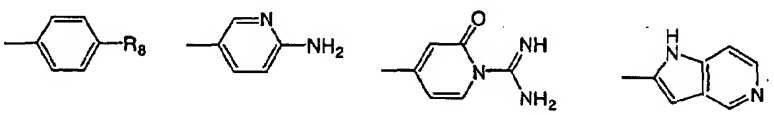
$$-CONH_2,$$

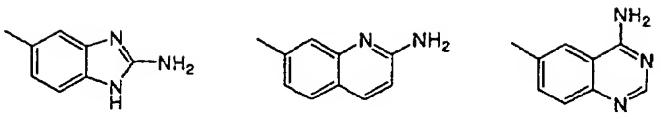


(wherein R_{12} represents a hydrogen atom or a methyl group) or

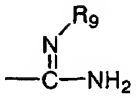


5. The compound according to any one of claims 1 to 4, wherein R_1 in Formula (1) is a group selected from the following formulae:





[wherein R_8 represents:



(wherein R_9 represents a hydrogen atom, an amino group, a hydroxy group, an acyl group, or an alkoxycarbonyl group having an optionally substituted linear or branched C_1-C_6 alkyl as its alkyl moiety)].

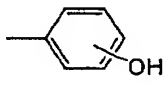
6. The compound according to any one of claims 1 to 5, wherein R_2 in Formula (1) is a hydrogen atom or a linear or branched C_1-C_3 alkyl group.

7. The compound according to any one of claims 1 to 6, wherein R_4 in Formula (1) is a hydrogen atom or a linear or branched C_1-C_3 alkyl group.

8. The compound according to any one of claims 1 to 6, wherein R_6 in Formula (1) is a hydrogen atom or a linear or branched C_1-C_3 alkyl group.

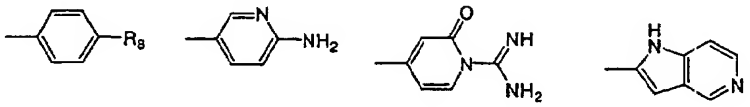
9. The compound according to claim 1, wherein R_3 in Formula (1) is $-(CH_2)_m-R_{11}$ (wherein m and R_{11} are as defined in claim 1).

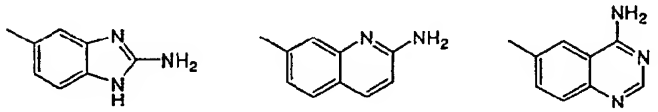
10. The compound according to claim 1, wherein in Formula (1), R_3 is a group of the following formula:



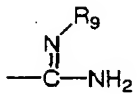
and R_7 is $-SO_2-R_{14}$ (wherein R_{14} is as defined in claim 1).

11. The compound according to claim 1, wherein in Formula (1),
R_1 is a group selected from the following formulae:





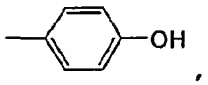
[wherein R_8 represents:



(wherein R_9 represents a hydrogen atom, an amino group, a hydroxy group, an acetyl group, a propionyl group, a butyryl group, an isobutyryl group, an isovaleryl group, a methoxycarbonyl group, an ethoxycarbonyl group, a t-butoxycarbonyl group or a benzyloxycarbonyl group)];

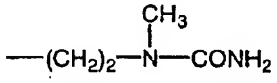
R_2 is a hydrogen atom or a methyl group;

R_3 is a group of the following formula:

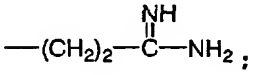


,

$-(CH_2)_2CONH_2$,



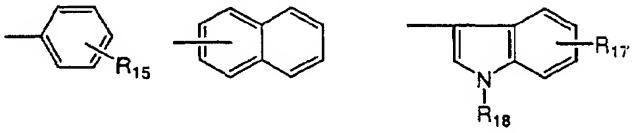
or



;

R_4 is a hydrogen atom or a methyl group;

R_5 is a linear or branched C_1-C_4 alkyl group or $-CH_2-R_{13}$ [wherein R_{13} represents a group selected from the following formulae:



(wherein

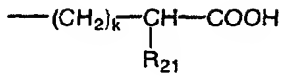
R_{15} represents a hydrogen atom, a t-butyl group, a methoxy group, a bromine atom, a chlorine atom, a benzoyl group, or a phenyl group which may be substituted with a methoxy group or a trifluoromethyl group or a nitro group or an amino group;

R_{17} represents a hydrogen atom, a hydroxy group, a methyl group, a linear or branched C_1-C_3 alkoxy group, $-O-(CH_2)_n-OH$ (wherein n represents an integer of 1 to 3), $-O-(CH_2)_p-COOH$ (wherein p represents an integer of 1 to 3), $-O-(CH_2)_q-NH_2$ (wherein q represents an integer of 1 to 3),$-OSO_2-R_{20}$ (wherein R_{20} represents an ethyl group, an n-propyl group, an i-propyl group or a benzyl group), a benzyloxy group, a 3- or 4-hydroxybenzyloxy group, or a 3- or 4-carboxybenzyloxy group; and

R_{18} represents a hydrogen atom, a methyl group, a methanesulfonyl group or a benzenesulfonyl group)];

R_6 is a hydrogen atom or a methyl group; and

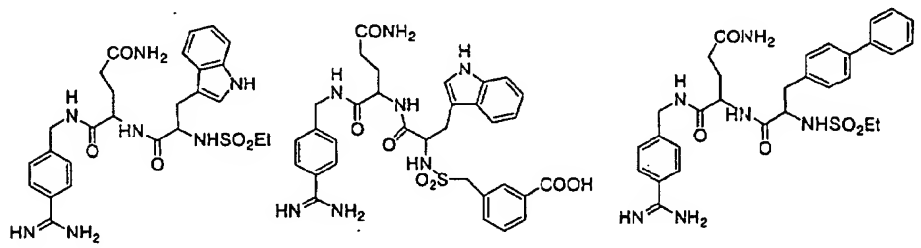
R_7 is a linear or branched C_1-C_4 alkyl group or a group of the following formula:

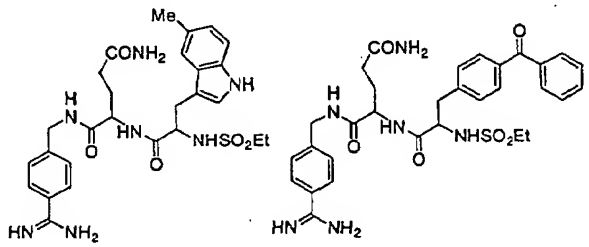


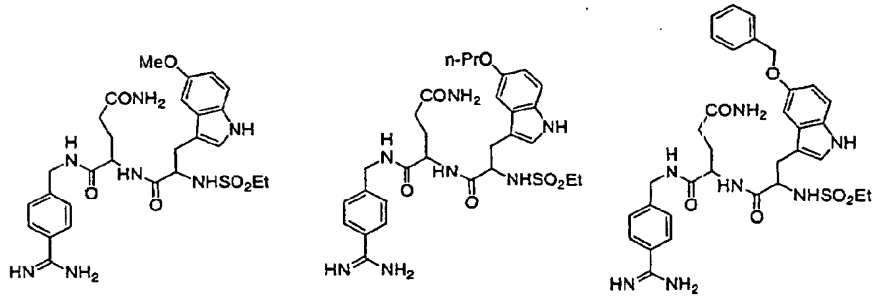
[wherein k represents an integer of 0 to 2, and R_{21} represents a hydrogen atom or -NHR_{22} (wherein R_{22} represents a methyl group or an acetyl group)] or

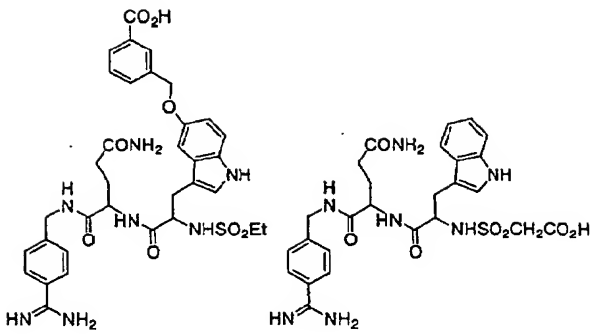
[wherein R_{14} represents a benzyl group, a 2-, 3- or 4-carboxybenzyl group, or an optionally substituted linear or branched C_1-C_4 alkyl group (wherein said alkyl group may be substituted with a carboxyl group or an alkoxycarbonyl group having a linear or branched C_1-C_3 alkyl as its alkyl moiety)].

12. The compound according to claim 1. which is selected from the following formulae:









13. A pharmaceutical composition comprising the compound according to claim 1.

14. An antithrombotic agent comprising the compound according to claim 1.

15. A blood coagulation factor VIIa inhibitor comprising the compound according to claim 1.

16. A crystal of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor.

17. The crystal according to claim 16, wherein the low-molecular weight reversible factor VIIa inhibitor is a compound of Formula (1) (wherein each symbol is as defined in claim 1).

18. A method for preparing a crystal of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, which comprises the following steps (i) to (iii):

(i) preparing human factor VIIa/human soluble tissue factor, which is co-crystallizable with the low-molecular weight reversible factor VIIa inhibitor;
(ii) preparing a concentrated sample for crystallization to add the low-molecular weight reversible factor VIIa inhibitor; and
(iii) obtaining the crystal of the complex: between human factor VIIa/human soluble tissue factor and the low-molecular weight reversible factor VIIa inhibitor from the concentrated sample for crystallization prepared in (ii) to add a seed crystal of a complex between a low-molecular weight irreversible or reversible factor VIIa inhibitor and human factor VIIa/human soluble tissue factor.

19. The method according to claim 18, wherein the low-molecular weight reversible factor VIIa inhibitor is a compound of Formula (1) (wherein each symbol is as defined in claim 1).

20. A medium carrying a part or all of structure coordinate data of a complex between human factor VIIa/human soluble tissue factor and a low-molecular weight reversible factor VIIa inhibitor, wherein said data are obtainable by X-ray crystal structure analysis of the crystal according to claim 16 or 17.

21. A method for computationally designing a low-molecular weight reversible factor VIIa inhibitor using the coordinate data according to claim 20.

22. The method according to claim 21, wherein the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with at least one of Asp60 side chain, Tyr94 side chain and Thr98 main chain of the human factor VIIa H chain.

23. The method according to claim 21, wherein the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with Lys192 side chain of the human factor VIIa H chain.

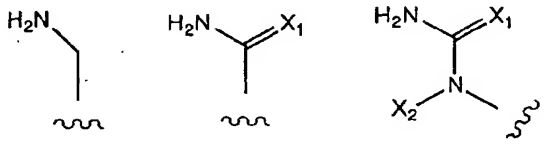
24. The method according to claim 21, wherein the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with at least one of Val170E, Gly170F, Asp170G, Ser170H, Pro17I and Gln217 of the human factor VIIa H chain.

25. The method according to claim 21, wherein the low-molecular weight reversible factor VIIa inhibitor is designed to have a substituent capable of interacting with the S4 subsite of the human factor VIIa H chain through a hole extending from the S4 site to the S4 subsite.

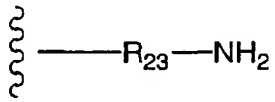
26. A low-molecular weight reversible factor VIIa inhibitor designed by the method according to any one of claims 21 to 25.

27. The low-molecular weight reversible factor VIIa inhibitor according to claim 26, which comprises any one of the partial structures shown in the following Class [A-1] or [A-2] as a partial structure capable of interacting with the S2 site of human factor VIIa:

Class [A-1]:



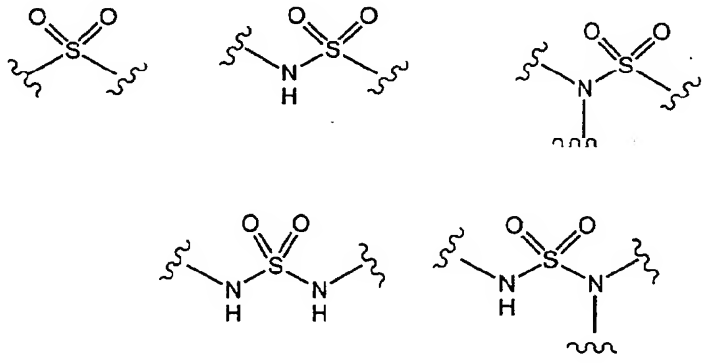
(wherein X_1 represents O or NH, and X_2 represents a hydrogen atom or a methyl group) or
Class [A-2]:



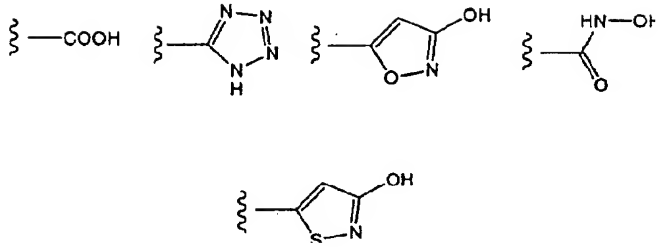
(wherein R_{23} represents a 6 or 5-membered aromatic ring containing a heteroatom(s)).

28. The low-molecular weight reversible factor VIIa inhibitor according to claim 26, which comprises any one of the partial structures shown in the following Class [B-1], [B-2], [B-3] or [B-4] as a partial structure capable of interacting with the S1 subsite of human factor VIIa:

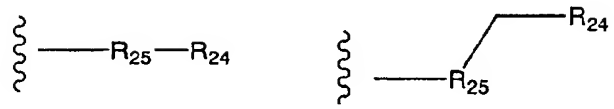
Class IB-1]:



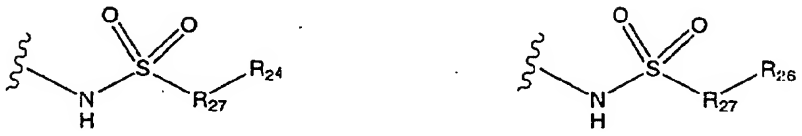
Class [B-2]:



Class [B-3]:



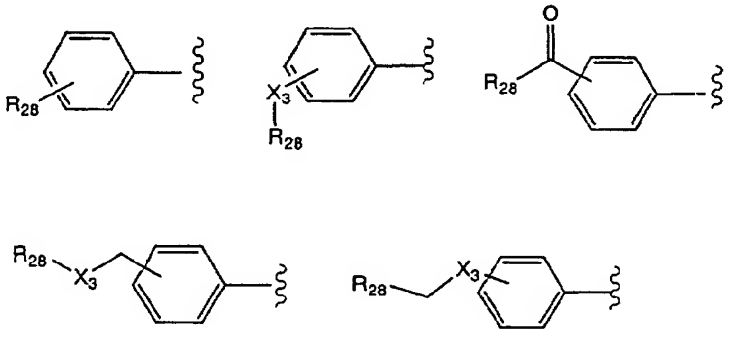
(wherein R_{24} represents the same partial structures defined as Class [B-2], and R_{25} represents a 6 or 5-membered aromatic ring containing a heteroatom(s))
Class [B-4]:



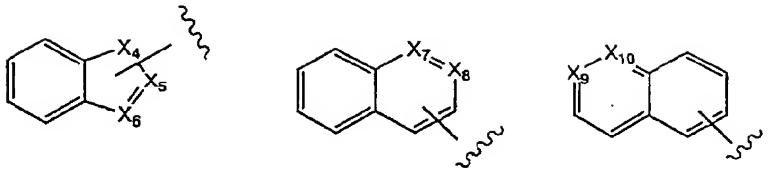
(wherein R_{27} represents a C_1-C_3 alkylene group, R_{24} represents the same partial structures defined as Class [B-2], and R_{26} represents the same partial structures defined as Class [B-3]).

29. The low-molecular weight reversible factor VIIa inhibitor according to claim 26, which comprises any one of the partial structures shown in the following Class [C-1] or [C-2] as a partial structure capable of interacting with the S4 site of human factor VIIa:

Class [C-1]:



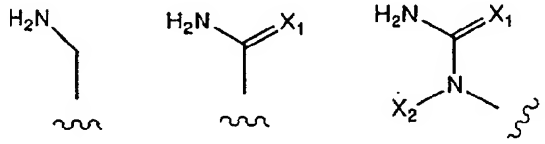
(wherein X_3 represents O, NH or CH_2, and R_{28} represents a 6 or 5-membered aromatic ring containing a heteroatom(s))
Class [C-2]:



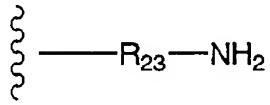
(wherein X_4 represents NH, S or O, and X_5, X_6, X_7, X_8, X_9 and X_{10} each independently represent N or CH).

30. The low-molecular weight reversible factor VIIa inhibitor according to claim 26, which comprises any one of the partial structures shown in the following Class [A-1] or [A-2] as a partial structure capable of interacting with the S2 site of human factor VIIa, any one of the partial structures shown in the following Class [B-1], [B-2], [B-3] or [B-4] as a partial structure capable of interacting with the S1 subsite, and any one of the partial structures shown in the following Class [C-1] or [C-2] as a partial structure capable of interacting with the S4 site:

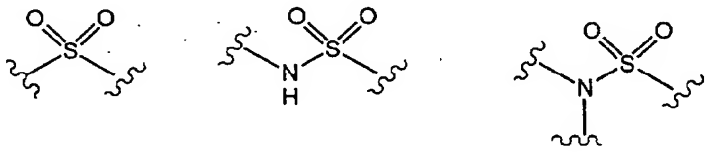
Class [A-1]:

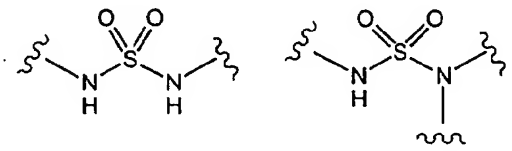


(wherein X_1 represents O or NH, and X_2 represents a hydrogen atom or a methyl group) or
Class [A-2]:

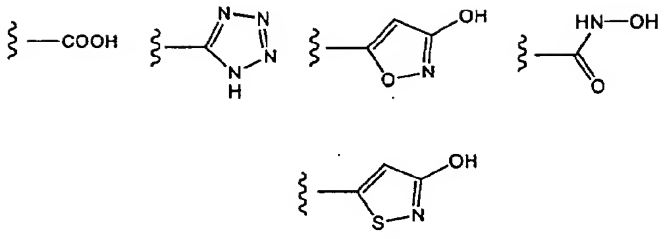


(wherein R_{23} represents a 6 or 5-membered aromatic ring containing a heteroatom(s));
Class [B-1]:

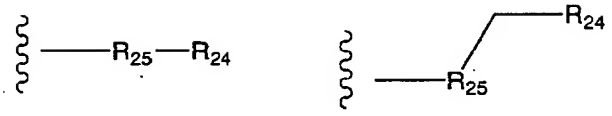




Class [B-2]:



Class [B-3]:

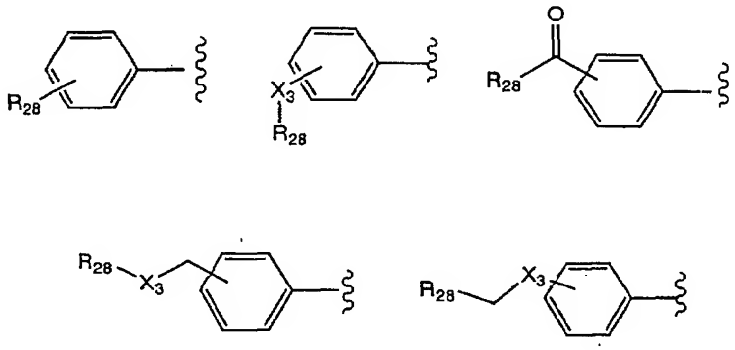


(wherein R_{24} represents the same partial structures defined as Class [B-2], and R_{25} represents a 6 or 5-membered aromatic ring containing a heteroatom(s))

Class [B-4]:

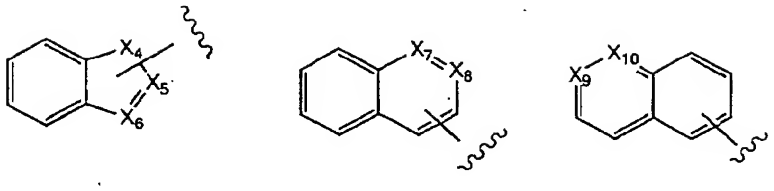
(wherein R_{27} represents a C_1-C_3 alkylene group, R_{24} represents the same partial structures defined as Class [B-2], and R_{26} represents the same partial structures defined as Class [B-3]); and

Class [C-1]:



(wherein X_3 represents O, NH or CH_2, and R_{28} represents a 6 or 5-membered aromatic ring containing a heteroatom(s))

Class [C-2]:



(wherein X_4 represents NH, S or O, and X_5, X_6, X_7, X_8, X_9 and X_{10} each independently represent N or CH).

Fig. 1

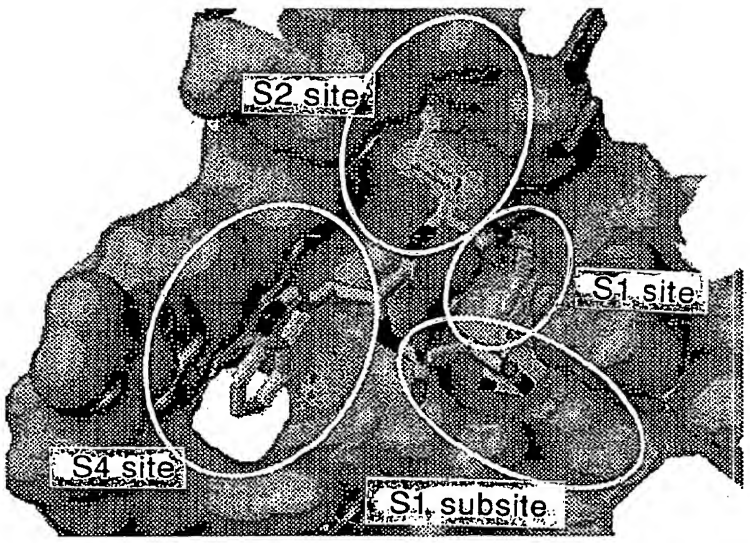


Fig. 2

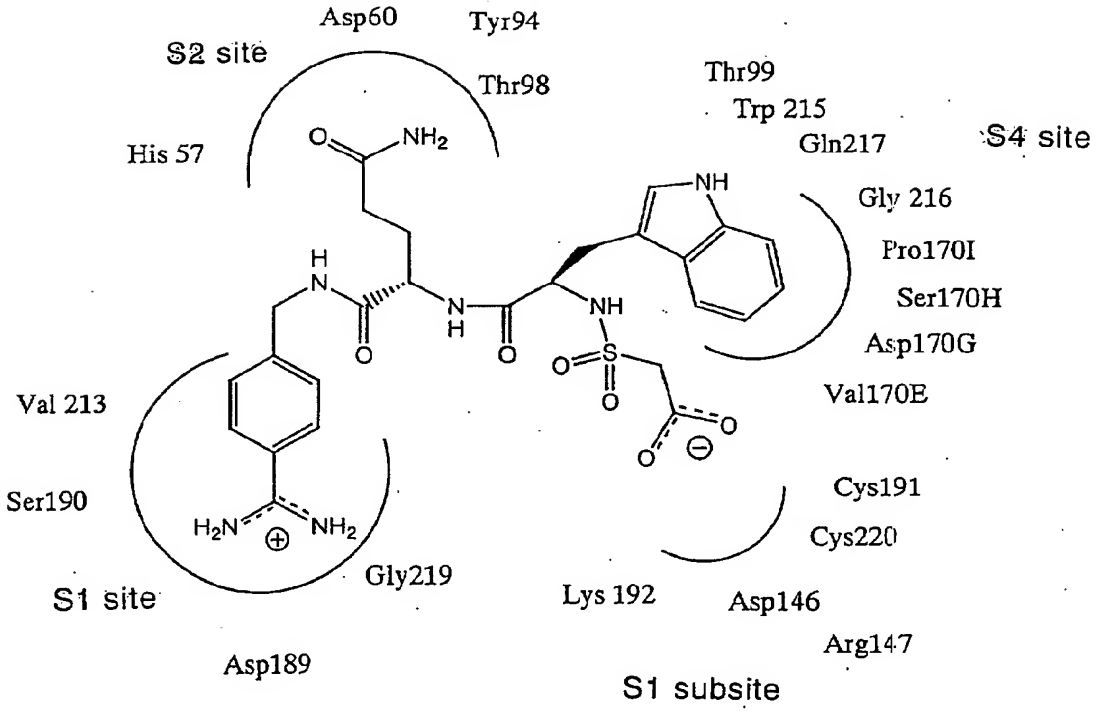
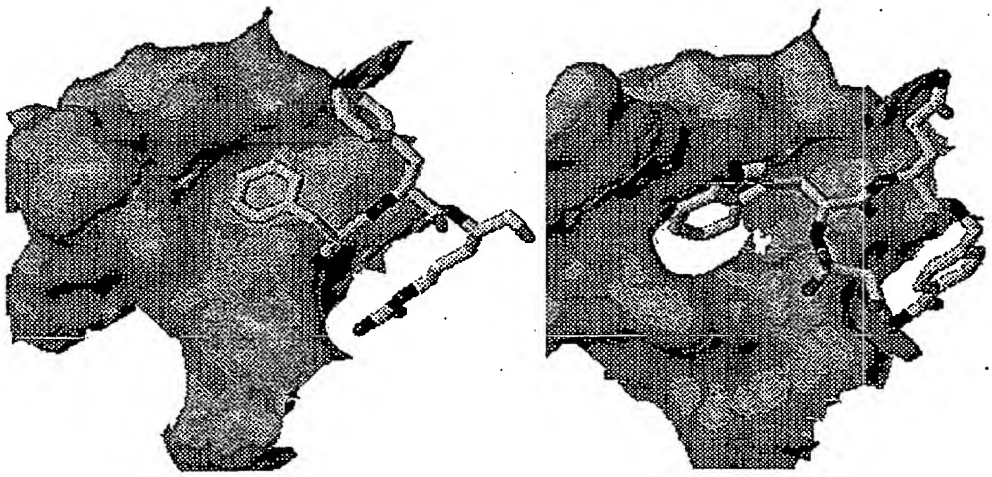

Asp60
Tyr94
S2 site
Thr98
Thr99
Trp 215
Gln217
S4 site
His 57
Gly 216
Pro170I
Ser170H
Asp170G
Val170E
Val 213
Ser190
Cys191
Cys220
S1 site
Gly219
Lys 192
Asp146
Arg147
Asp189
S1 subsite

Fig. 3



INTERNATIONAL SEARCH REPORT

International application No.
PCT/JP02/00883

A. CLASSIFICATION OF SUBJECT MATTER
Int.Cl[7] C07K5/062, C07K5/065, C07K5/078, C07K14/745, G01N33/15, G01N33/68, G06F17/50

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
Int.Cl[7] C07K5/062, C07K5/065, C07K5/078, C07K14/745, G01N33/15, G01N33/68, G06F17/50

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
REGISTRY(STN), CA(STN), MEDLINE(STN), WPI(DIALOG), BIOSIS(DIALOG)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 00/75172 A2 (Aventis Pharma Deut GmbH.), 14 December, 2000 (14.12.00), & EP 1059302 A1 & AU 200053976 A & CZ 200104357 A3 & NO 200106005 A & BR 200011461 A & EP 1189929 A2	1-30
A	WO 00/58346 A1 (Sanofi-Synthelabo), 05 October, 2000 (05.10.00), & FR 2791683 A1 & AU 200033017 A	1-30
A	WO 00/41531 A2 (Genentech), 20 July, 2000 (20.07.00), & EP 1144373 A2 & AU 200033451 A & NO 200103462 A & CZ 200102508 A3	1-30

☒ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

* Special categories of cited documents:
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"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
10 May, 2002 (10.05.02)	21 May, 2002 (21.05.02)
Name and mailing address of the ISA/ Japanese Patent Office	Authorized officer
Facsimile No.	Telephone No.

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INTERNATIONAL SEARCH REPORT

International application No.
PCT/JP02/00883

C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	WO 00/15658 A1 (Aventis Pharma Deut GmbH.), 23 March, 2000 (23.03.00), & EP 987274 A1 & AU 9959723 A & NO 200101293 A & BR 9913742 A & CZ 200100914 A3 & EP 1114061 A1 & US 6287794 B1 & KR 2001075130 A & ZA 200101861 A	1-30
A	DENNIS, M. S. et al., Peptide exosite inhibitors of factor VIIa as anticoagulants. Nature 2000, Vol.404, No.6777, pages 465 to 470	1-30
A	PIKE, A. C. et al., Structure of human factor VIIa and its implications for the triggering of blood coagulation. Proc. Natl. Acad. Sci. USA. 1999, Vol.96, No.16, pages 8925 to 8930	1-30

Form PCT/ISA/210 (continuation of second sheet) (July 1998)